

Supporting Information

Iron-Mediated Radical Halo-Nitration of Alkenes

Tsuyoshi Taniguchi, Tatsuya Fujii and Hiroyuki Ishibashi*

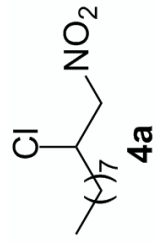
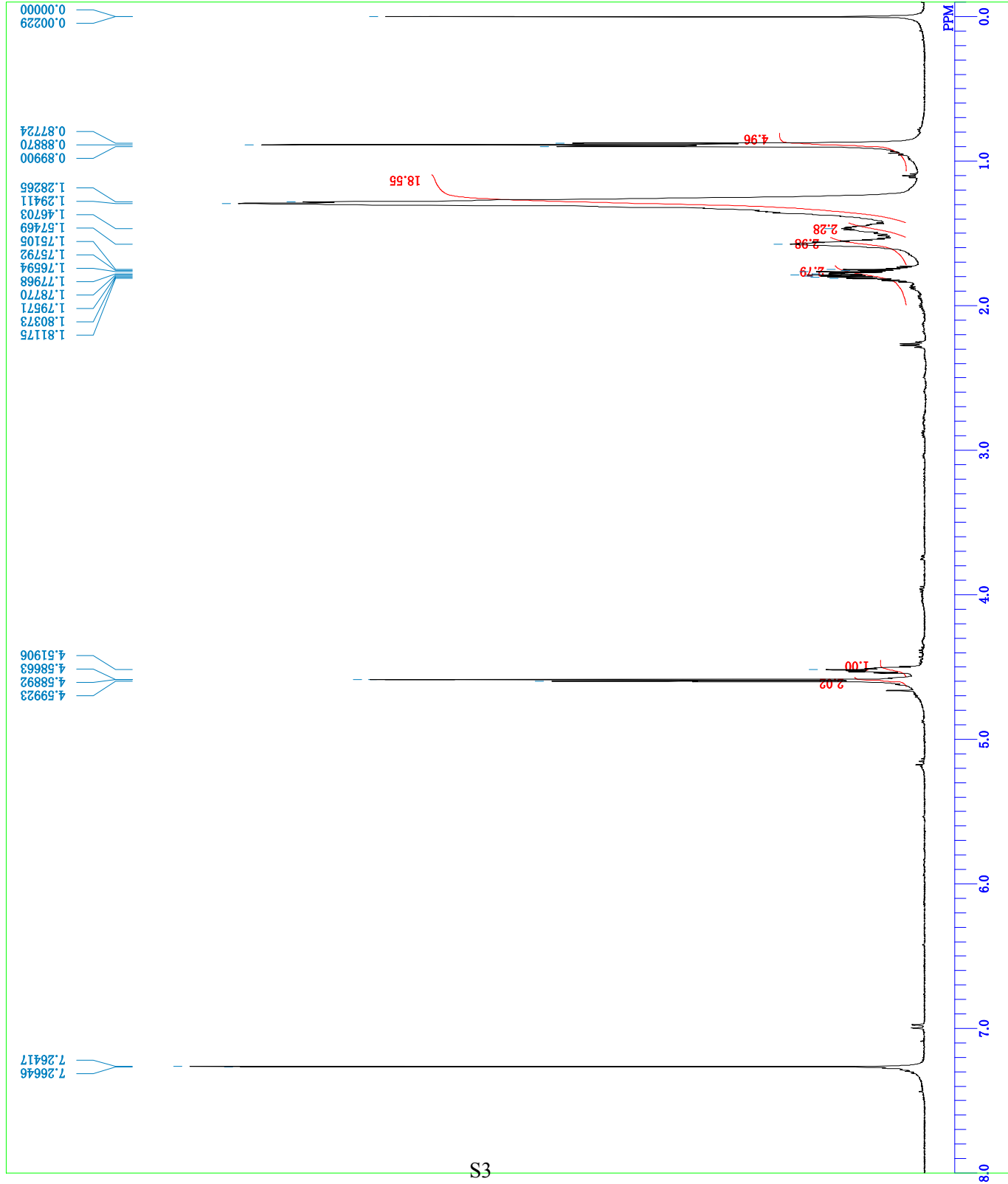
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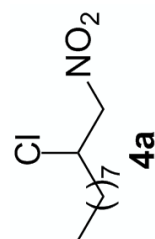
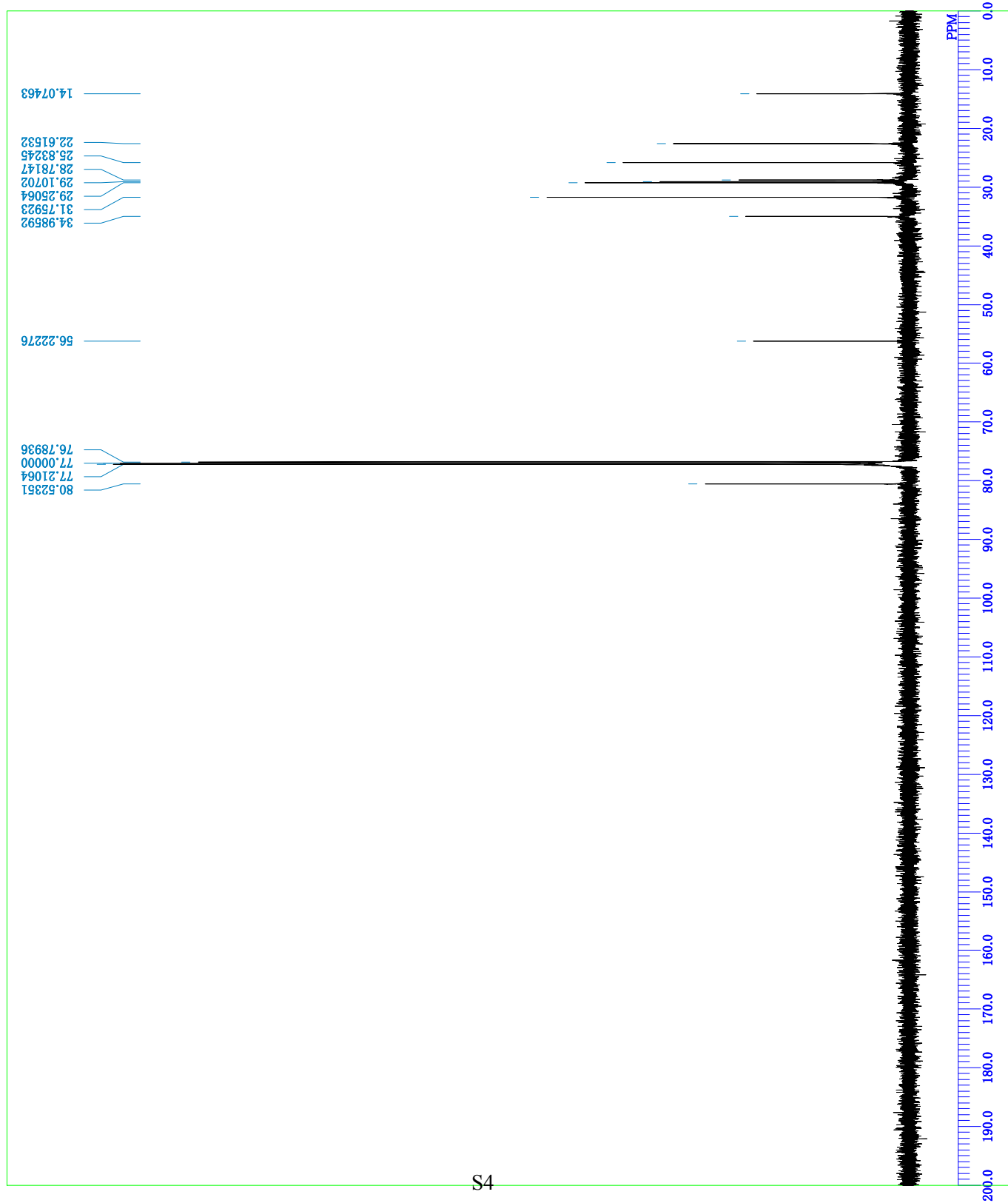
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4a-1H.als
 100114
 14-01-2010 21:49:42
 1H
 single pulse, ex2
 600.17 MHz
 5.30 KHz
 5.47 Hz
 13107
 9008.87 Hz
 16
 1.4549 sec
 2.0000 sec
 5.40 usec
 1H 16.7 c
 CDCL3
 0.00 ppm
 0.12 Hz
 46
 RGAIN

DFILE
 COMINT
 DATUM
 OBNUC
 EXMOD
 OBFREQ
 OBSETT
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

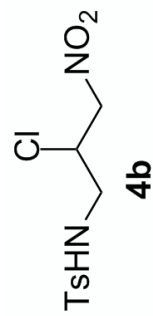
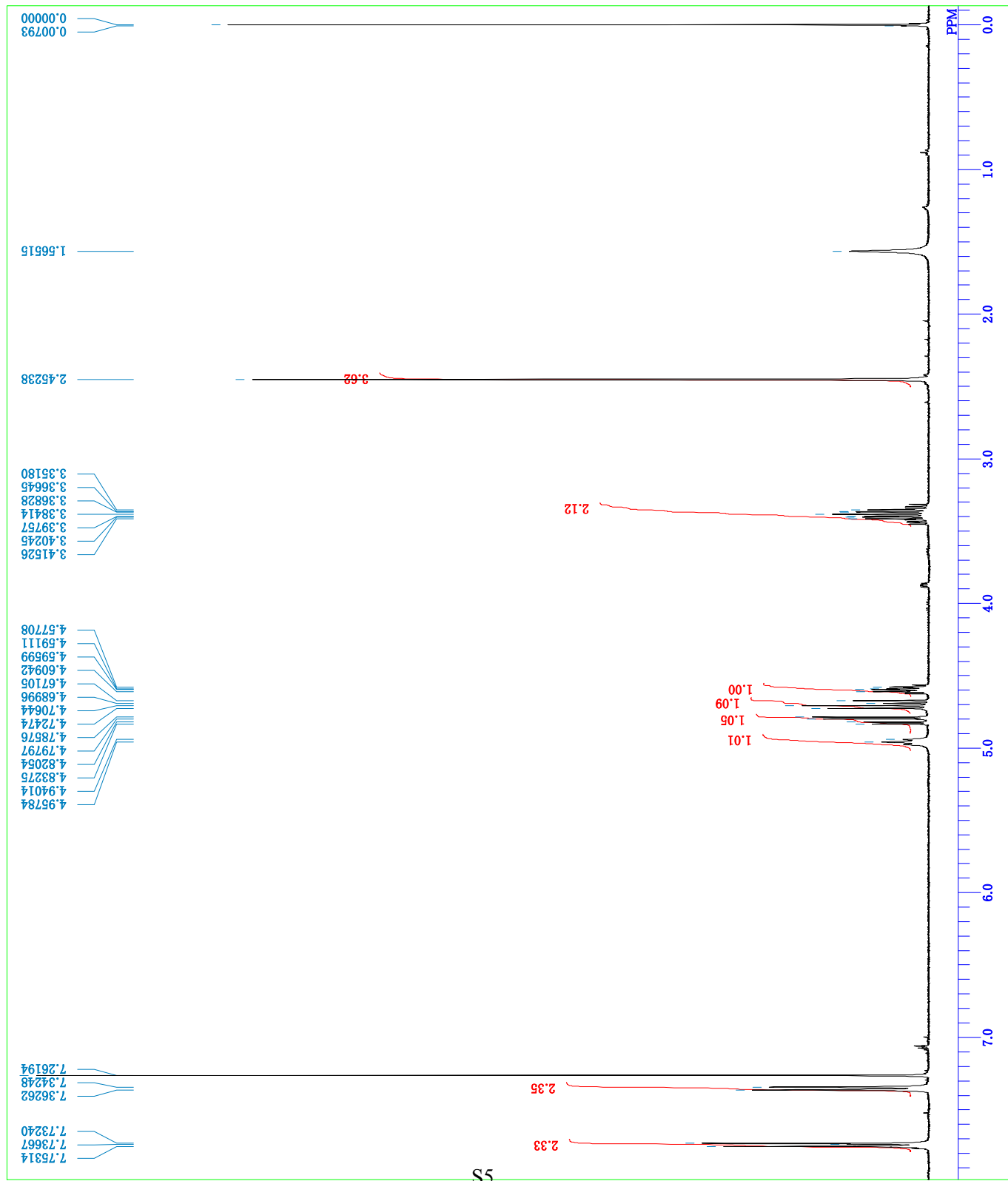


4a-C.als
100115
15-01-2010 20:57:03
13C
single pulse dec
OBMOD 150.92 MHz
OBFRQ 8.52 KHz
OBSET 1.74 Hz
OBFIN 26214
POINT 37878.21 Hz
FREQ 273
SCANS 0.6921 sec
ACQTM 1.2000 sec
PD 2.77 usec
PW1 1H
IRNUC 17.9 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF BF
RGAIN 0.25 Hz
54



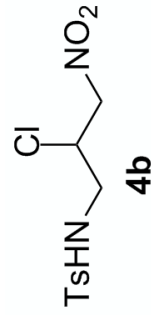
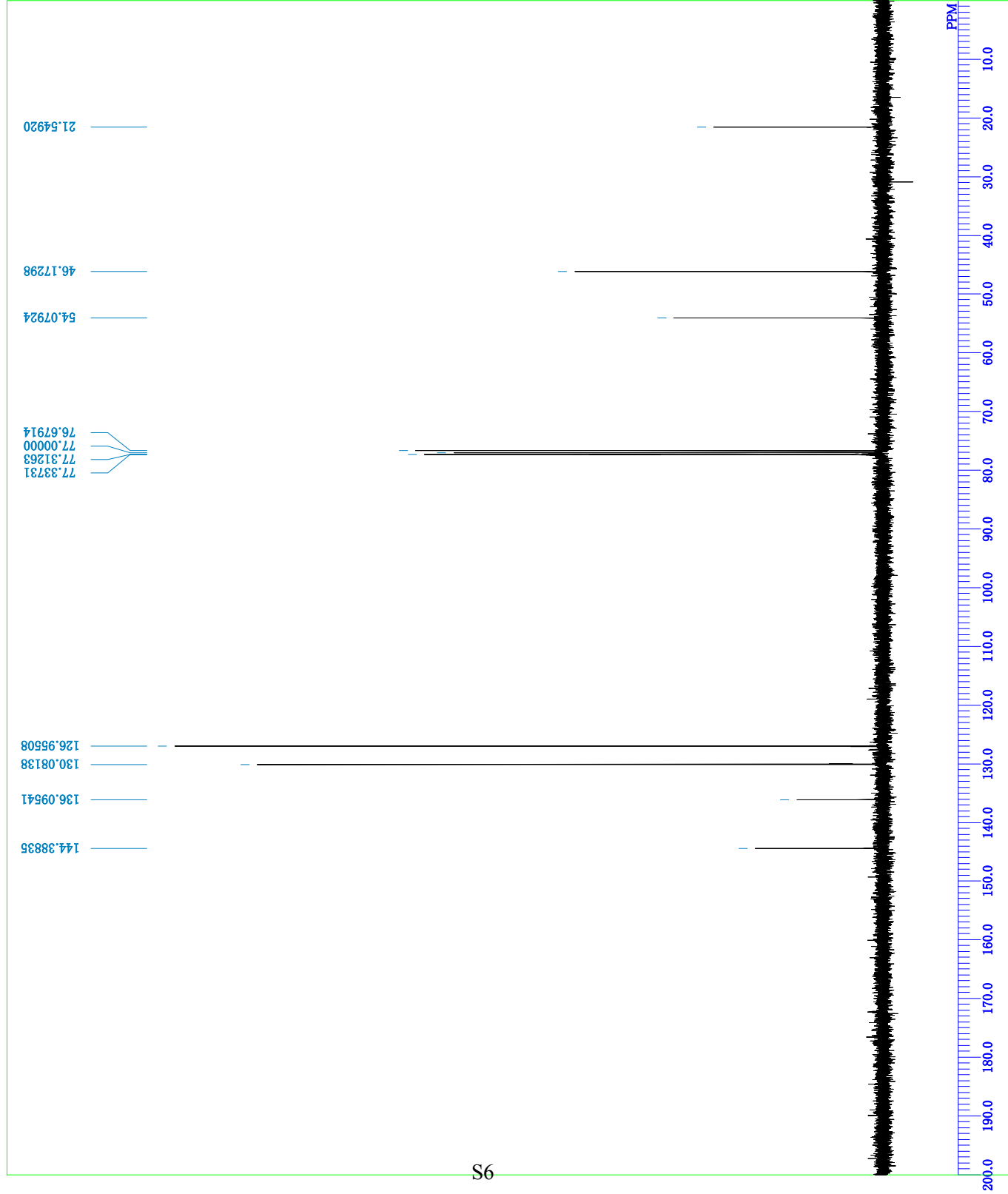
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COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

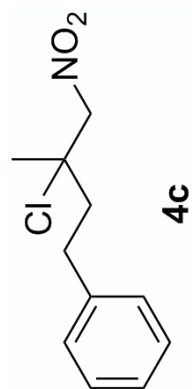
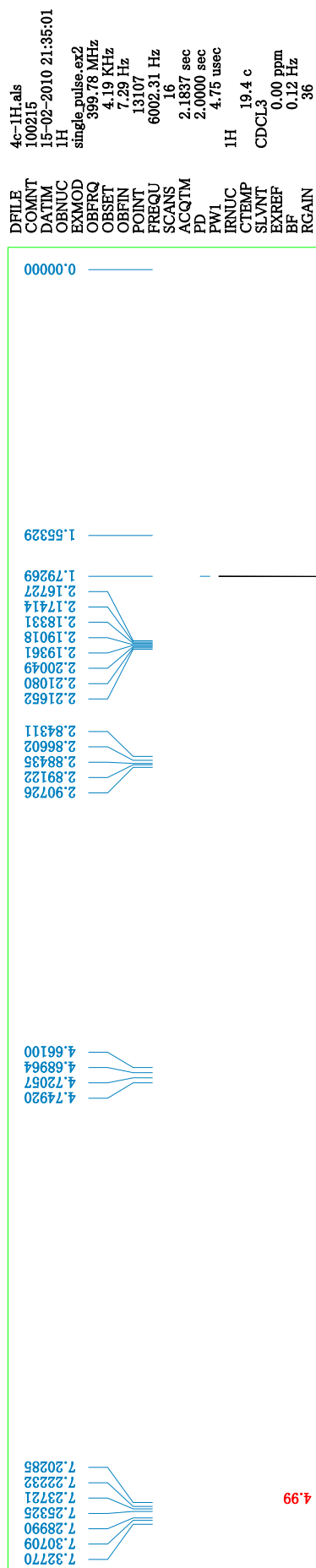
4b-1H.als
09123
Wed Dec 02 13:46:49 2009
1H
non
399.65 MHz
0.00 KHz
134300.00 Hz
32768
7993.60 Hz
16
4.0993 sec
2.9007 sec
6.80 usec
1H
22.4 c
CDCL3
0.00 ppm
0.12 Hz
28



4b-C:als
091130
Mon Nov 30 22:19:52 2009
13C
bcm
100.40 MHz
0.00 KHz
135500.00 Hz
32768
27100.27 Hz
257
1.2091 sec
1.7909 sec
4.90 usec
1H
23.2 c
CDCL3
77.00 ppm
0.12 Hz
26
RGAIN

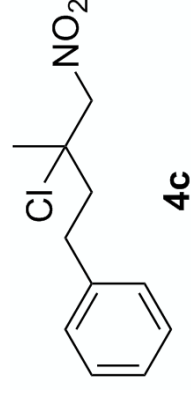
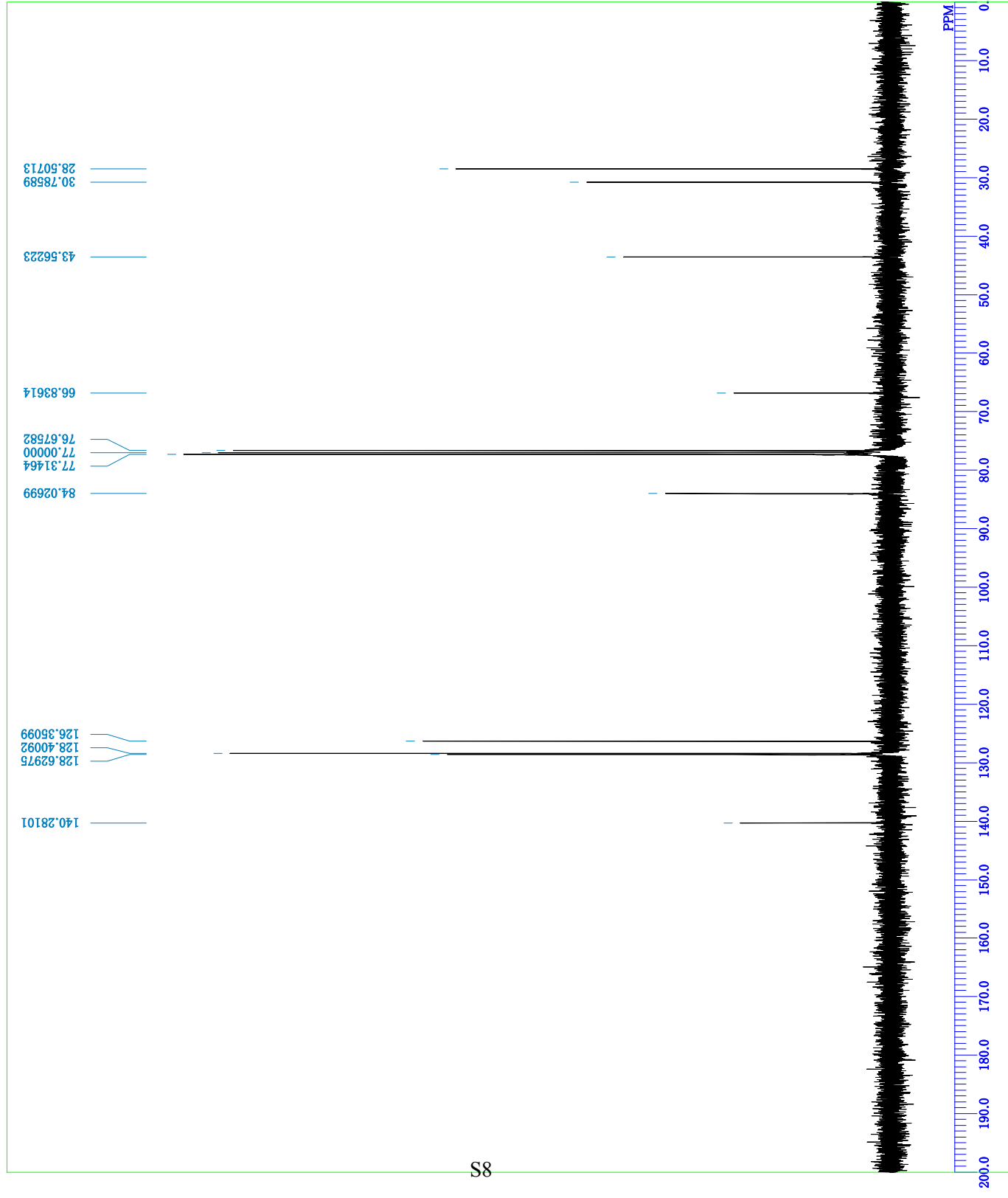
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



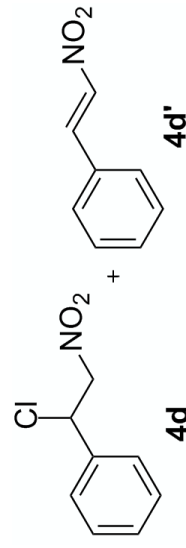
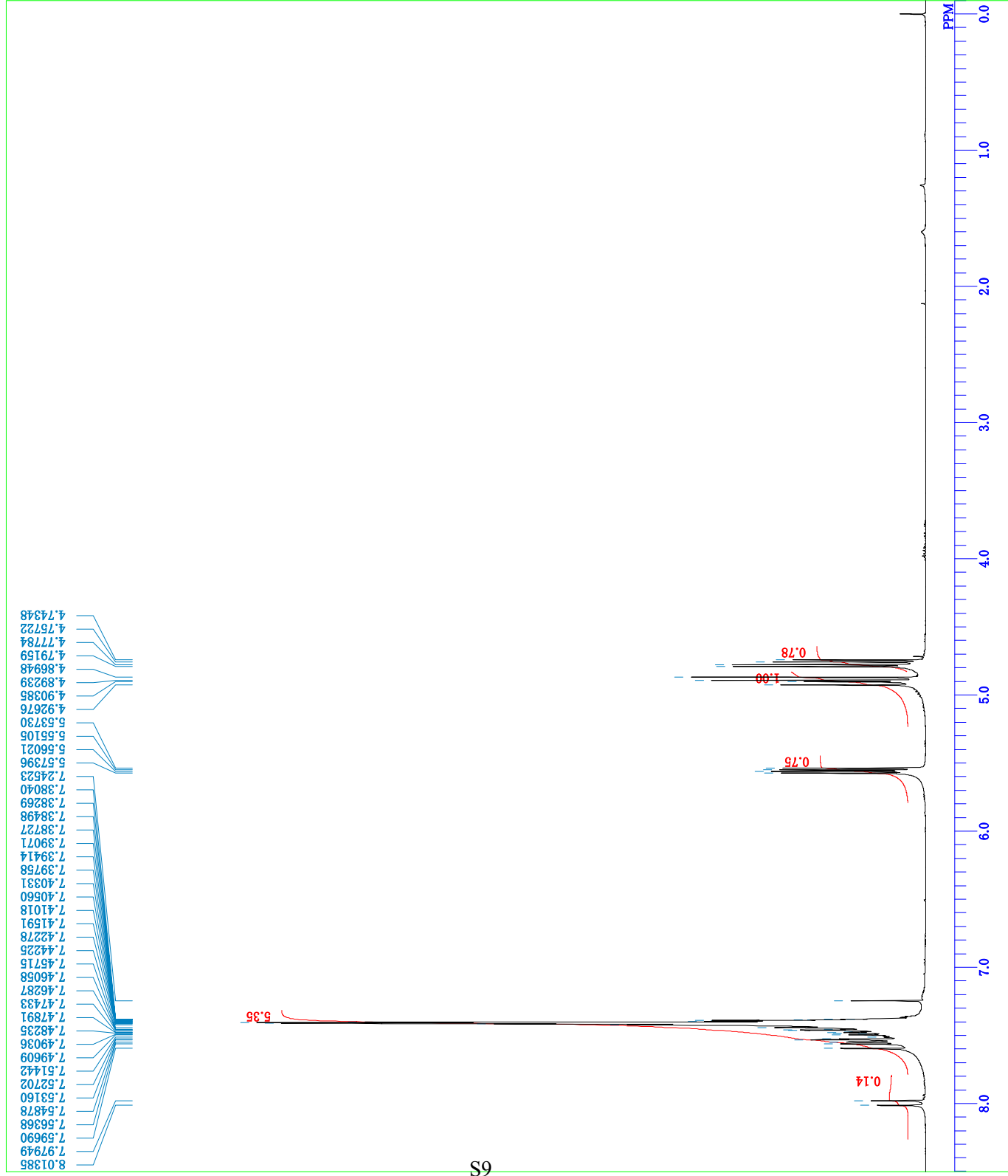


4c-C.als
100215
15-02-2010 21:47:31
13C
single pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.24 Hz
323
1.0433 sec
1.2000 sec
2.87 usec
1H 19.7 c
CDCL3
77.00 ppm
0.12 Hz
60
RGAIN

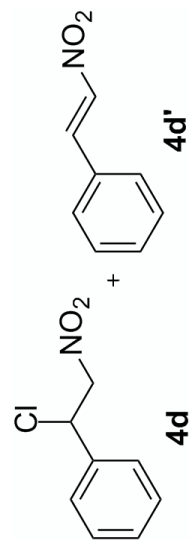
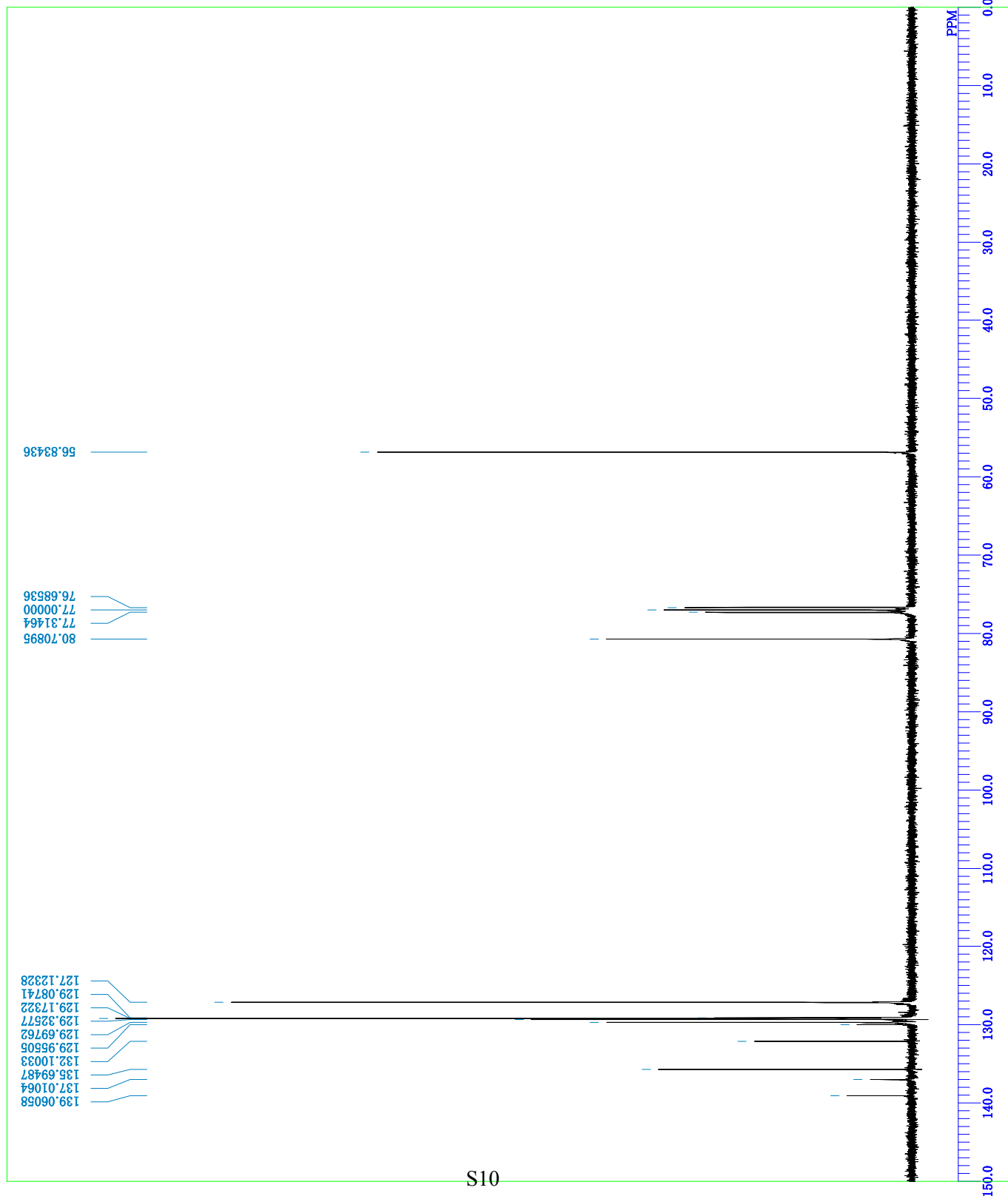
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



DFILE 4d-1H.als
 COMINT 100123
 DATIM 23-01-2010 16:10:33
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSETT 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.31 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 2.0000 sec
 PW1 4.75 usec
 IRNUC 1H
 CTEMP 19.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30



4d-C.als
100123
23-01-2010 16:27:60
13C
single_pulse_dec
EXMOD 100.53 MHz
OBFRQ 5.35 KHz
OBSET 5.86 Hz
POINT 26214
FREQ 25125.24 Hz
SCANS 451
ACQTM 1.0433 sec
PD 1.2000 sec
PW1 2.87 usec
IRNUC 1H 19.6 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF BF 0.00 Hz
RGAIN 60

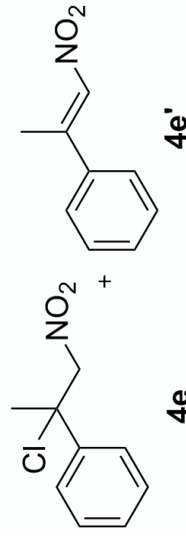
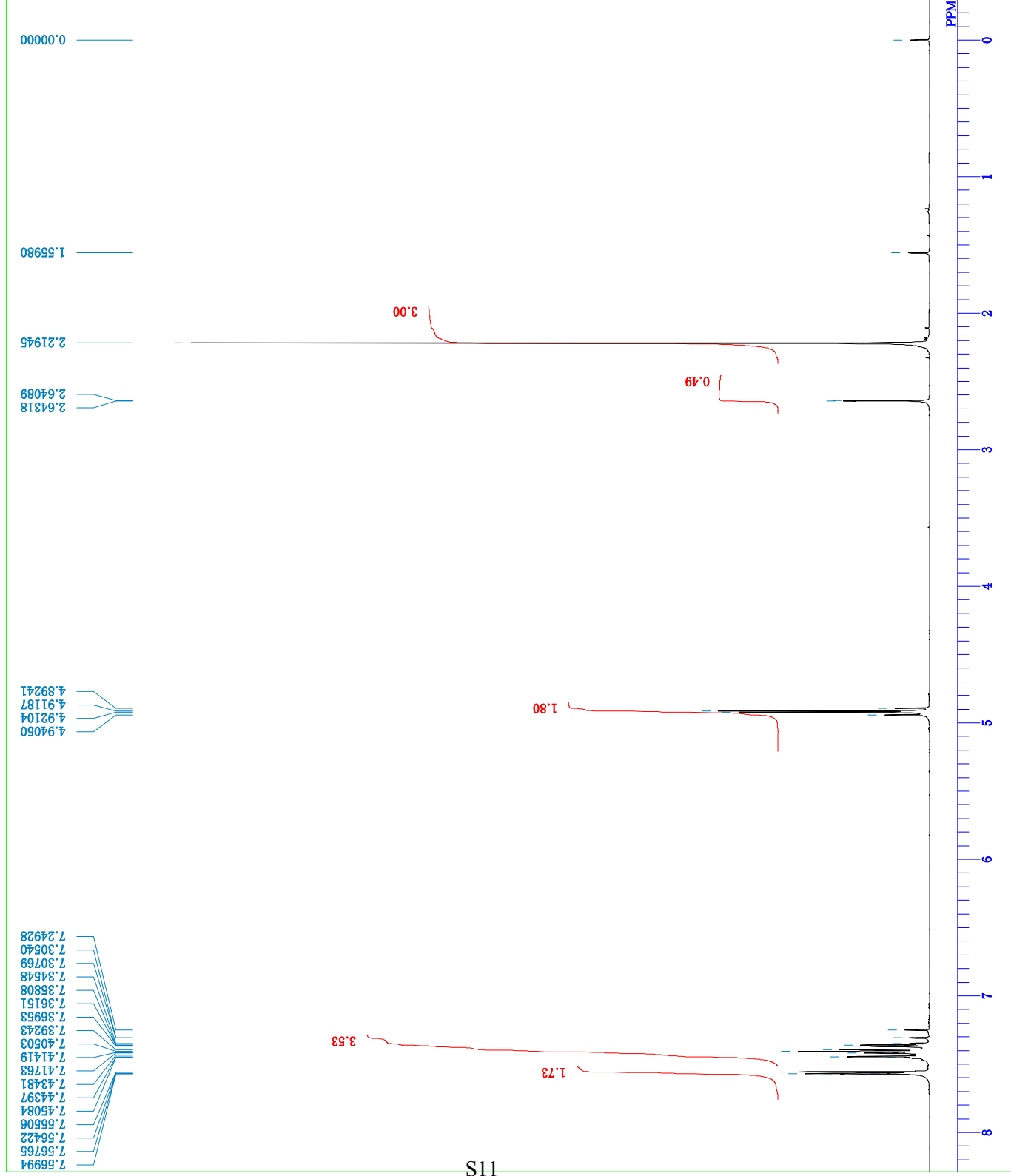


115

4e-H1als
100303
03-03-2010 22:04:07
1H
single pulse, ex2
600.17 MHz
5.30 KHz
5.47 Hz
13107
9008.87 Hz
16
1.4549 sec
2.0000 sec
6.50 usec
1H
19.8 c
CDCL3
0.00 ppm
0.25 Hz
34

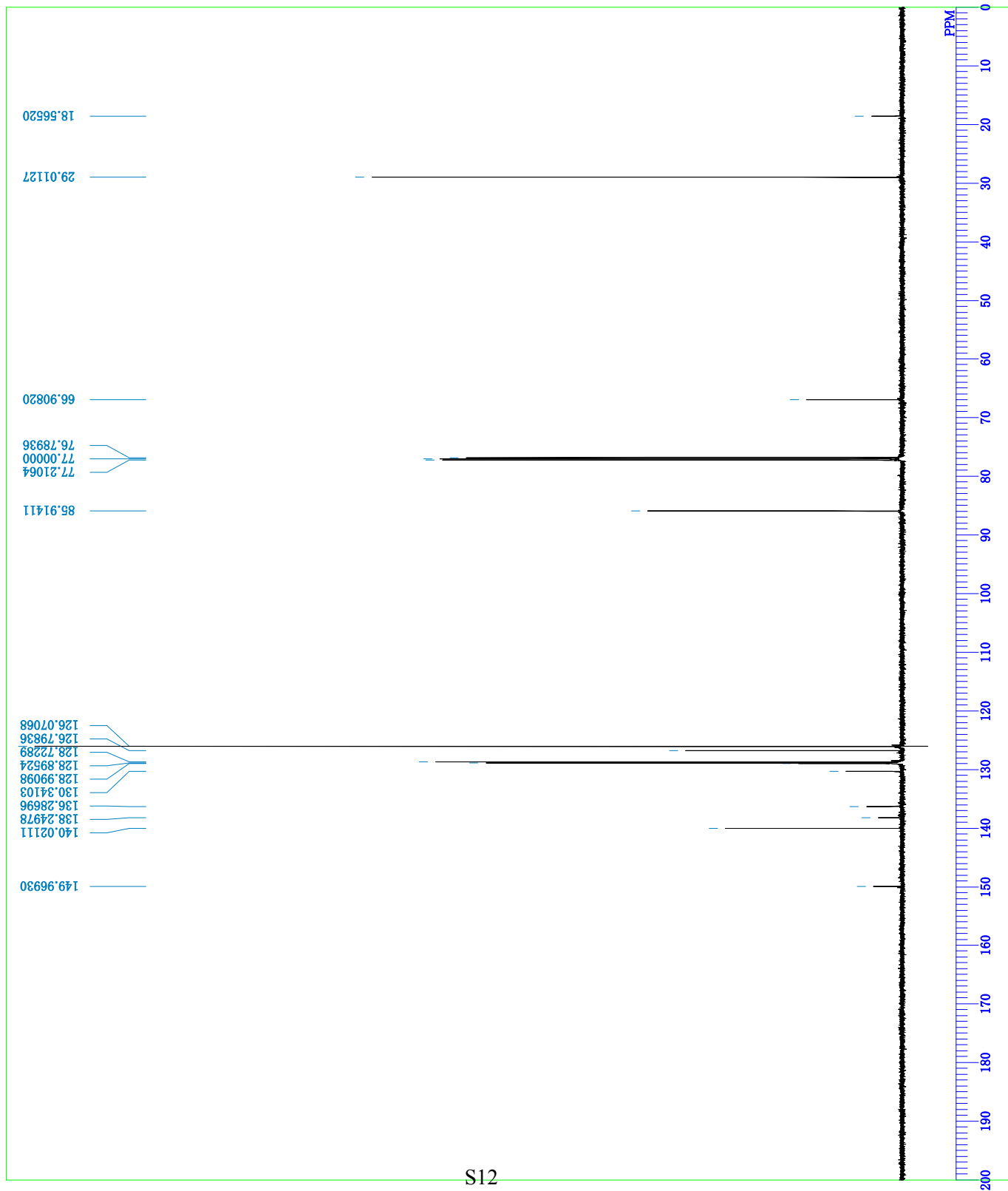
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

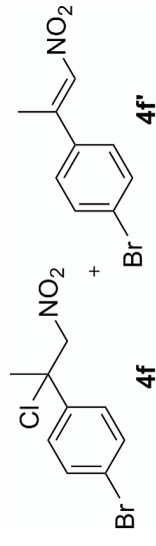
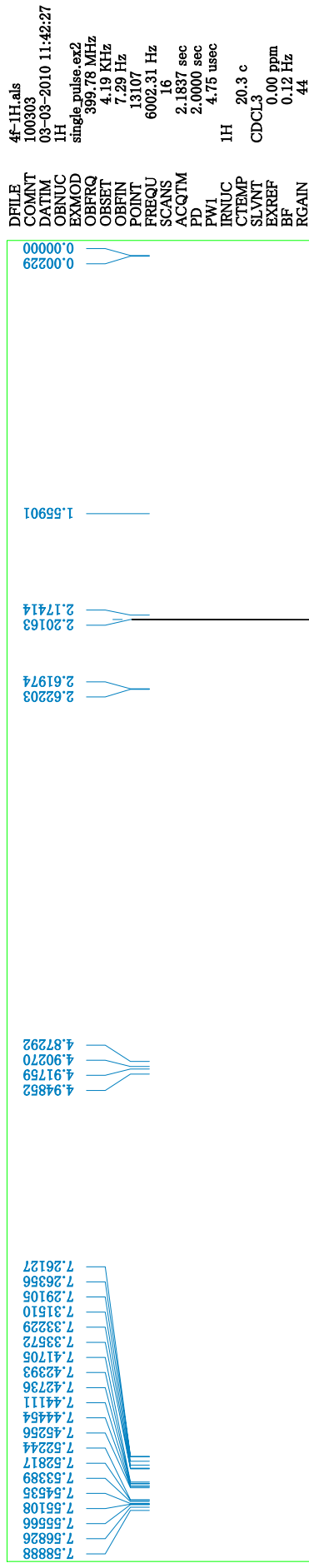
0.00000
1.55980
2.21945
2.64089
2.64318
4.89241
4.91187
4.92104
4.94050
7.24928
7.30540
7.30769
7.34548
7.35808
7.36151
7.36953
7.39243
7.40603
7.41419
7.41763
7.43481
7.44397
7.45084
7.55006
7.56422
7.56765
7.56994



4e-C:als
 100303
 03-03-2010 22:47:48
 13C
 single_pulse dec
 150.92 MHz
 8.52 KHz
 1.74 Hz
 26214
 37878.21 Hz
 1371
 0.6921 sec
 1.2000 sec
 4.00 usec
 1H
 20.7 c
 CDCL3
 77.00 ppm
 0.25 Hz
 56
 RGAIN

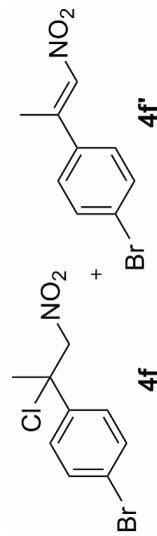
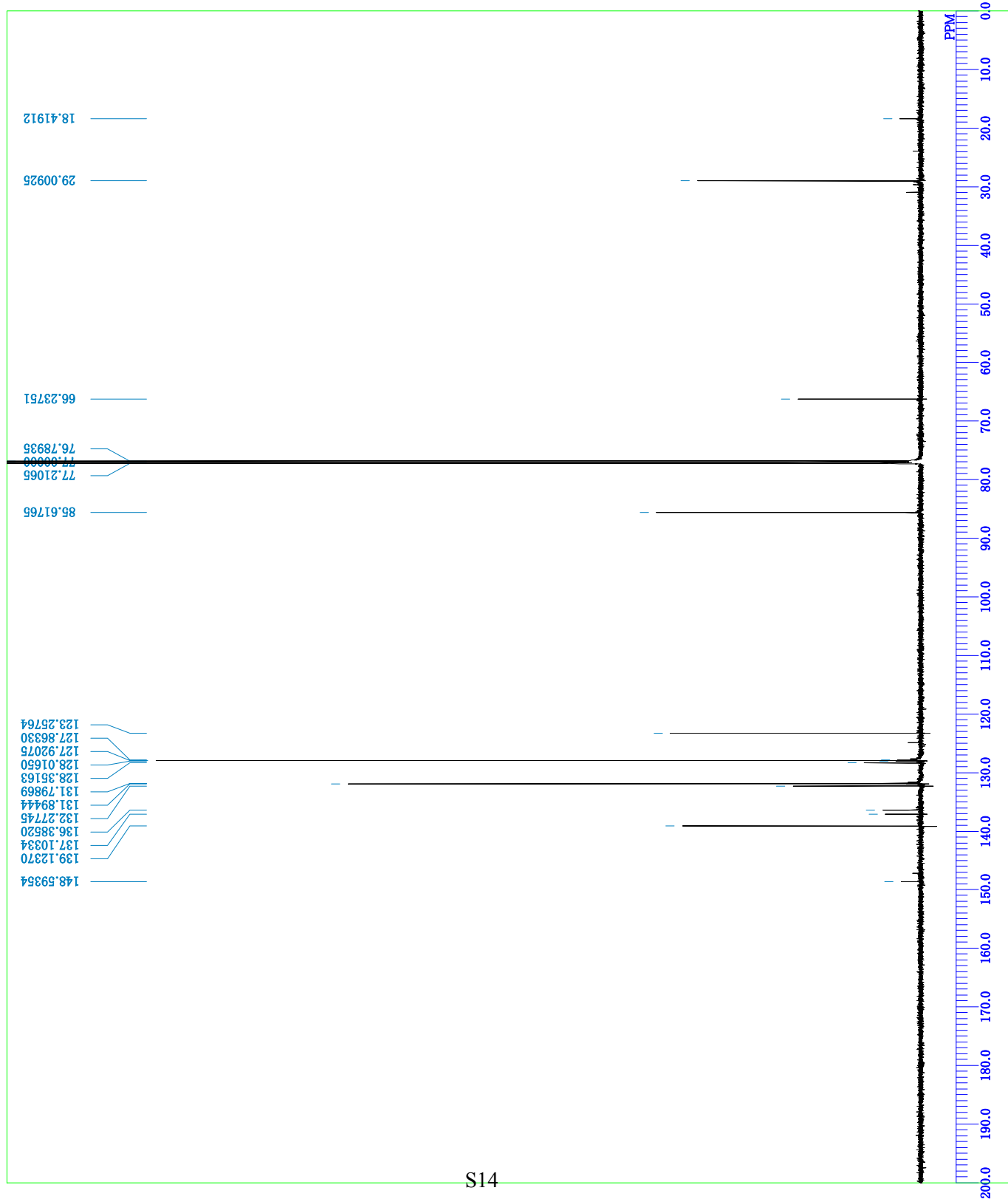
DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN





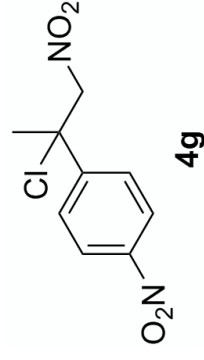
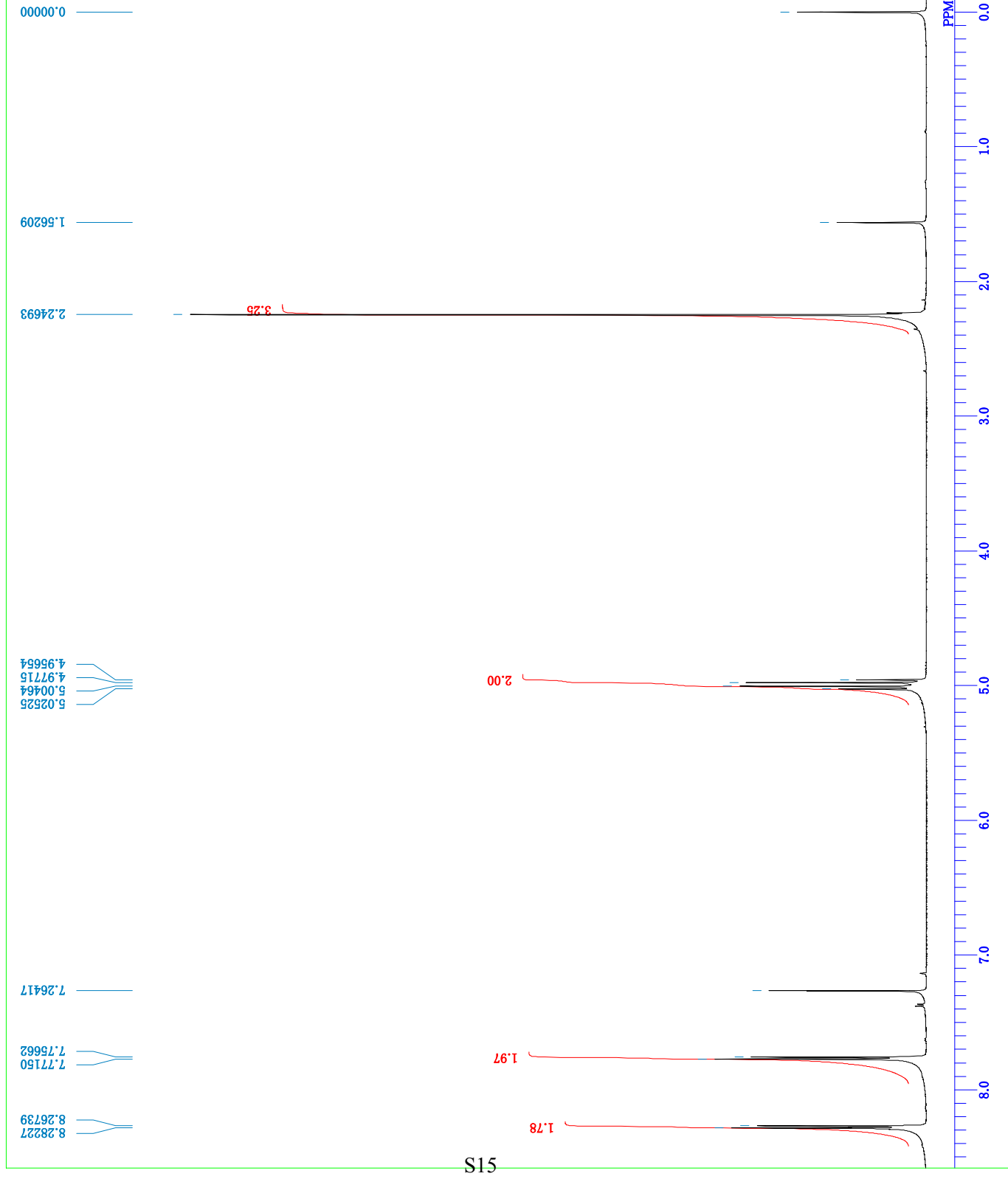
4f-C.als
 100303
 04-03-2010 08:50:02
 13C
 single pulse dec
 150.92 MHz
 8.52 KHz
 1.74 Hz
 20970
 30302.11 Hz
 18561
 0.6921 sec
 1.2000 sec
 PD
 4.00 usec
 PW1
 1H
 20.4 c
 CDCL3
 77.00 ppm
 0.12 Hz
 56
 RGAIN

DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

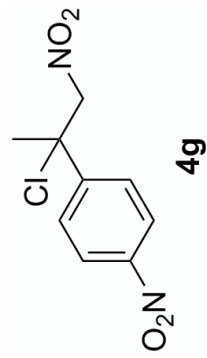
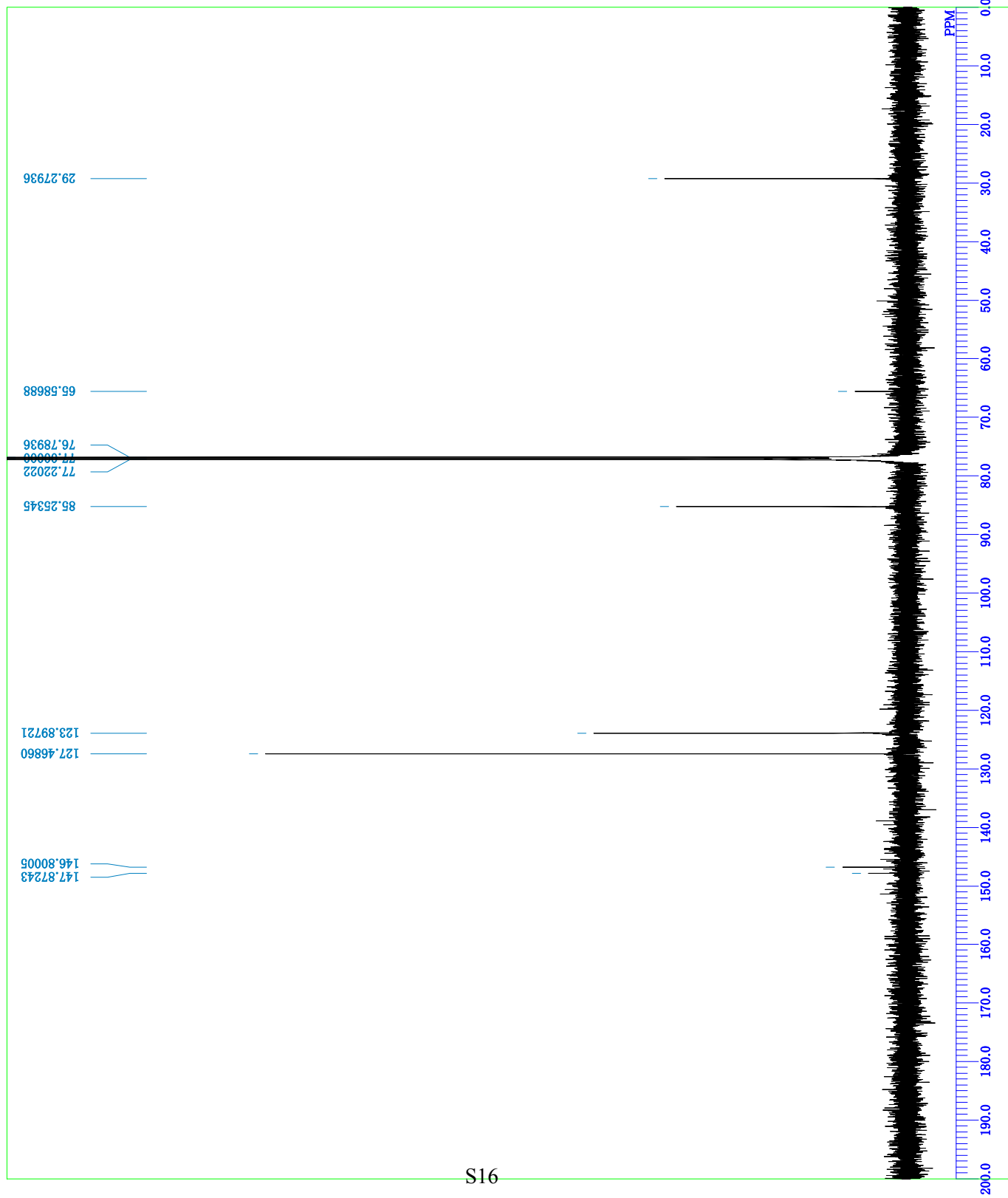


DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

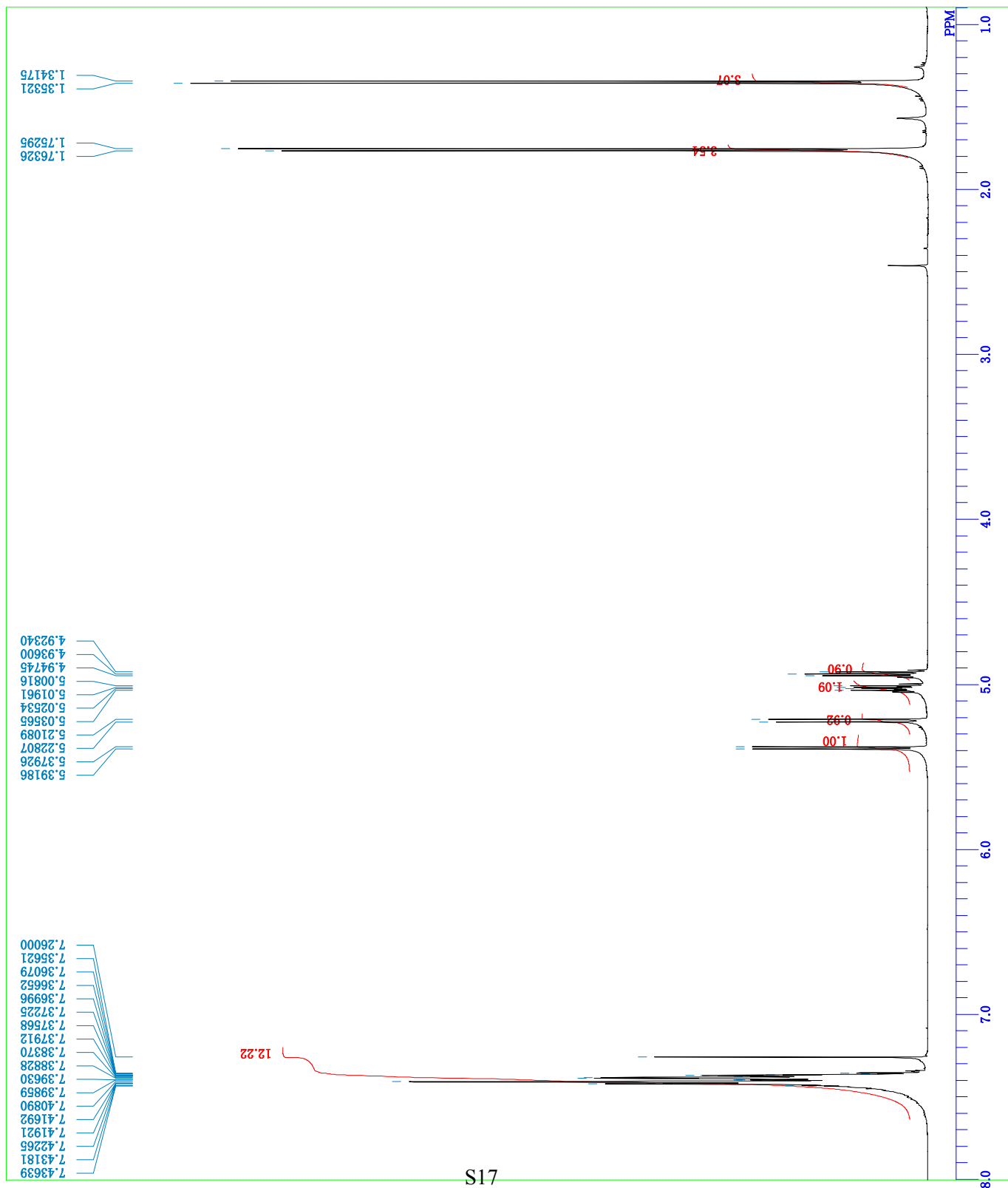
4g-1H.als
100112
12-01-2010 16:22:06
1H
single pulse, ex2
600.17 MHz
5.30 KHz
5.47 Hz
13107
9008.87 Hz
16
1.4549 sec
2.0000 sec
5.40 usec
1H
18.4 c
CDCL3
0.00 ppm
0.25 Hz
48



4g-C.als
100112
12-01-2010 17:02:11
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
512
0.6921 sec
1.2000 sec
2.77 usec
1H
19.1 c
CDCL3
77.00 ppm
0.25 Hz
52
RGAIN

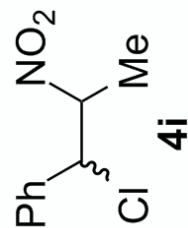
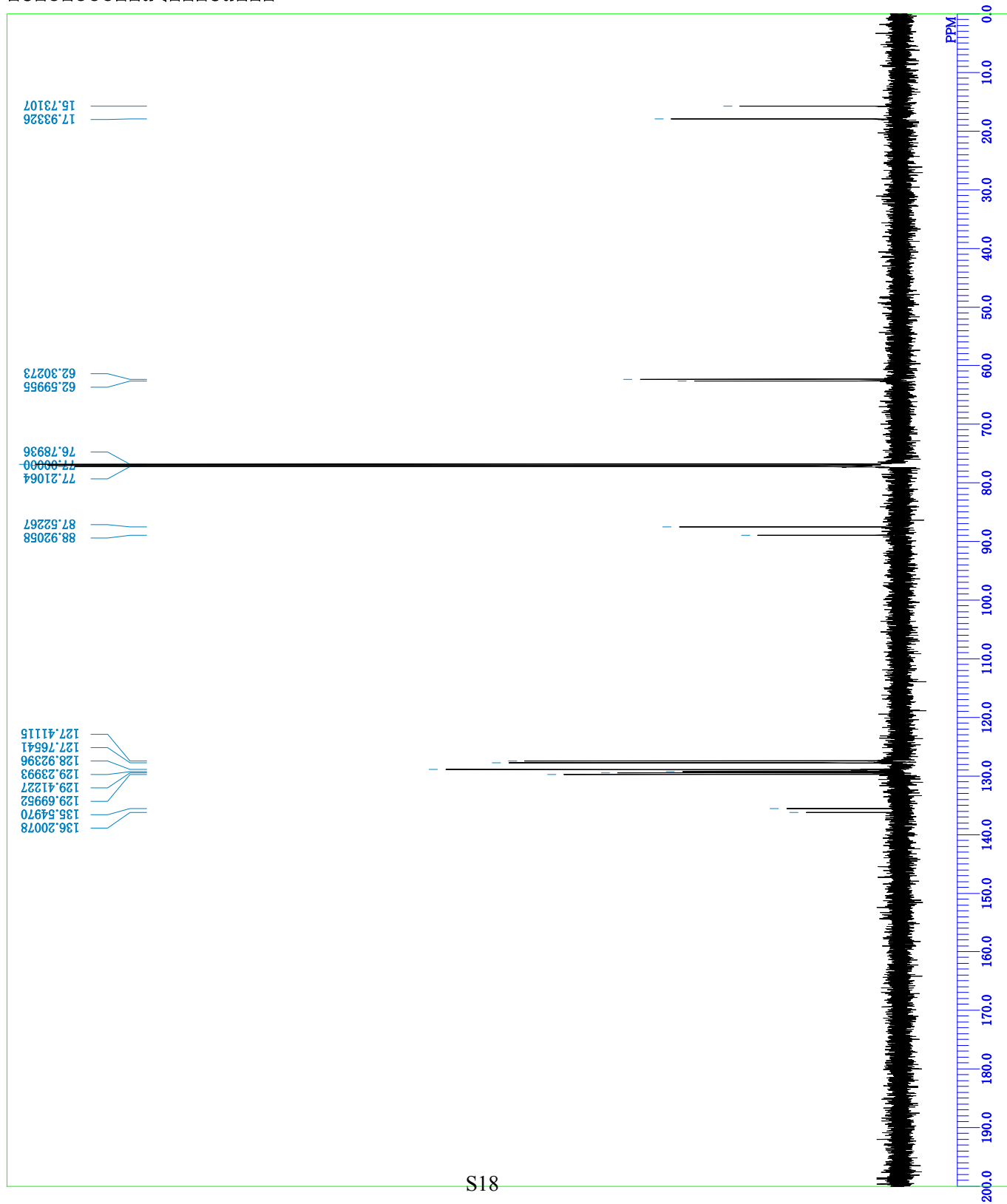


4i-1H.als
 100212
 12-02-2010 20:35:13
 1H
 single pulse, ex2
 600.17 MHz
 5.30 KHz
 5.47 Hz
 8387
 5765.50 Hz
 16
 1.4549 sec
 2.0000 sec
 6.50 usec
 1H 18.7 c
 CDCL3
 7.26 ppm
 0.12 Hz
 38
 RGAIN

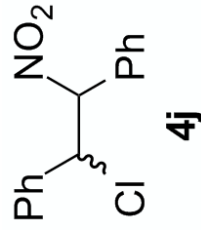
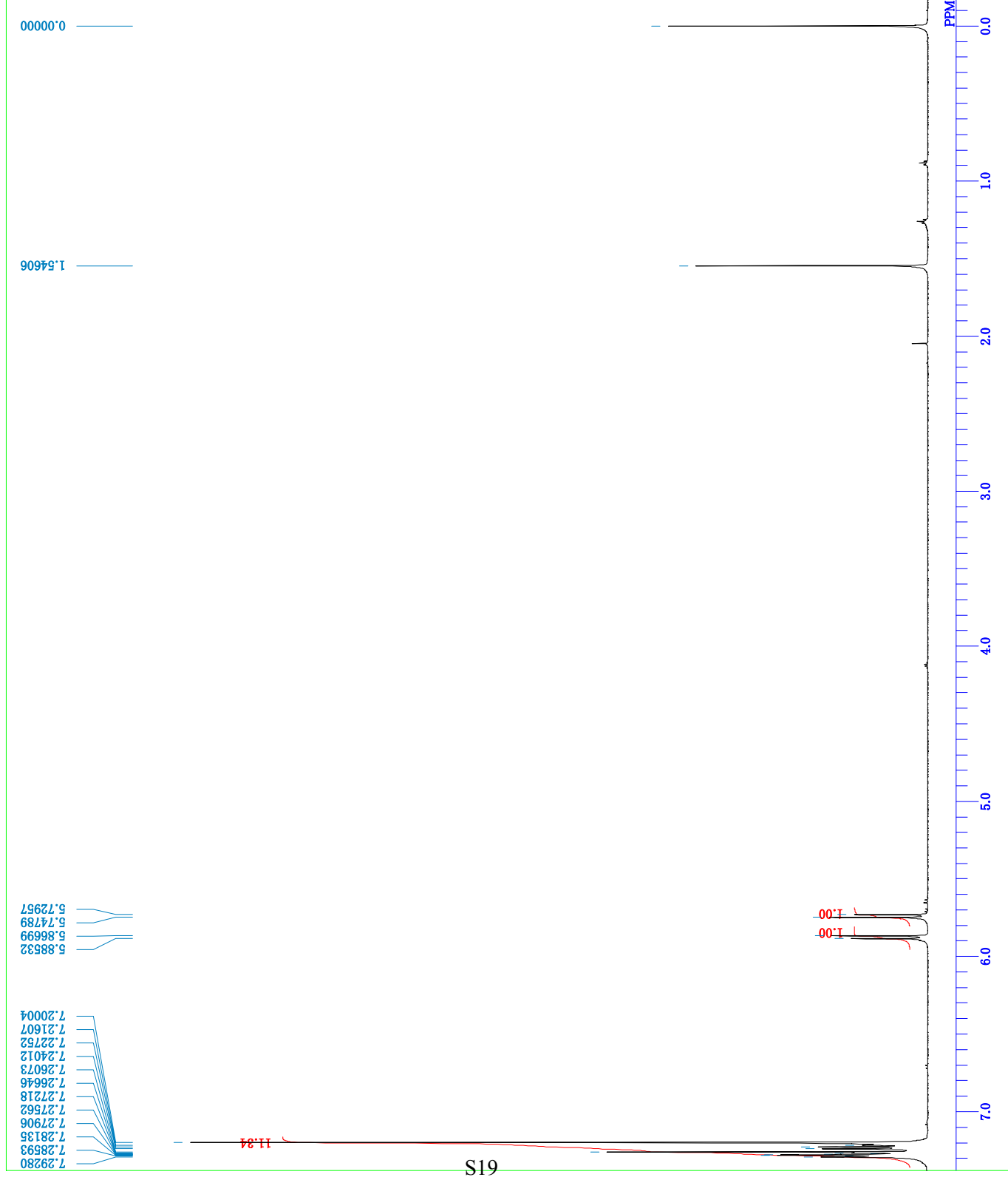


4i-C.als
100212
12-02-2010 20:43:51
13C
single_pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
258
0.6921 sec
1.2000 sec
4.00 usec
1H 19.6 c
CDCL3
77.00 ppm
0.12 Hz
56
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWL
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

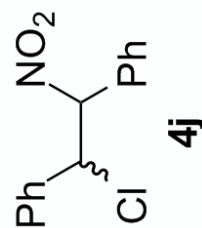
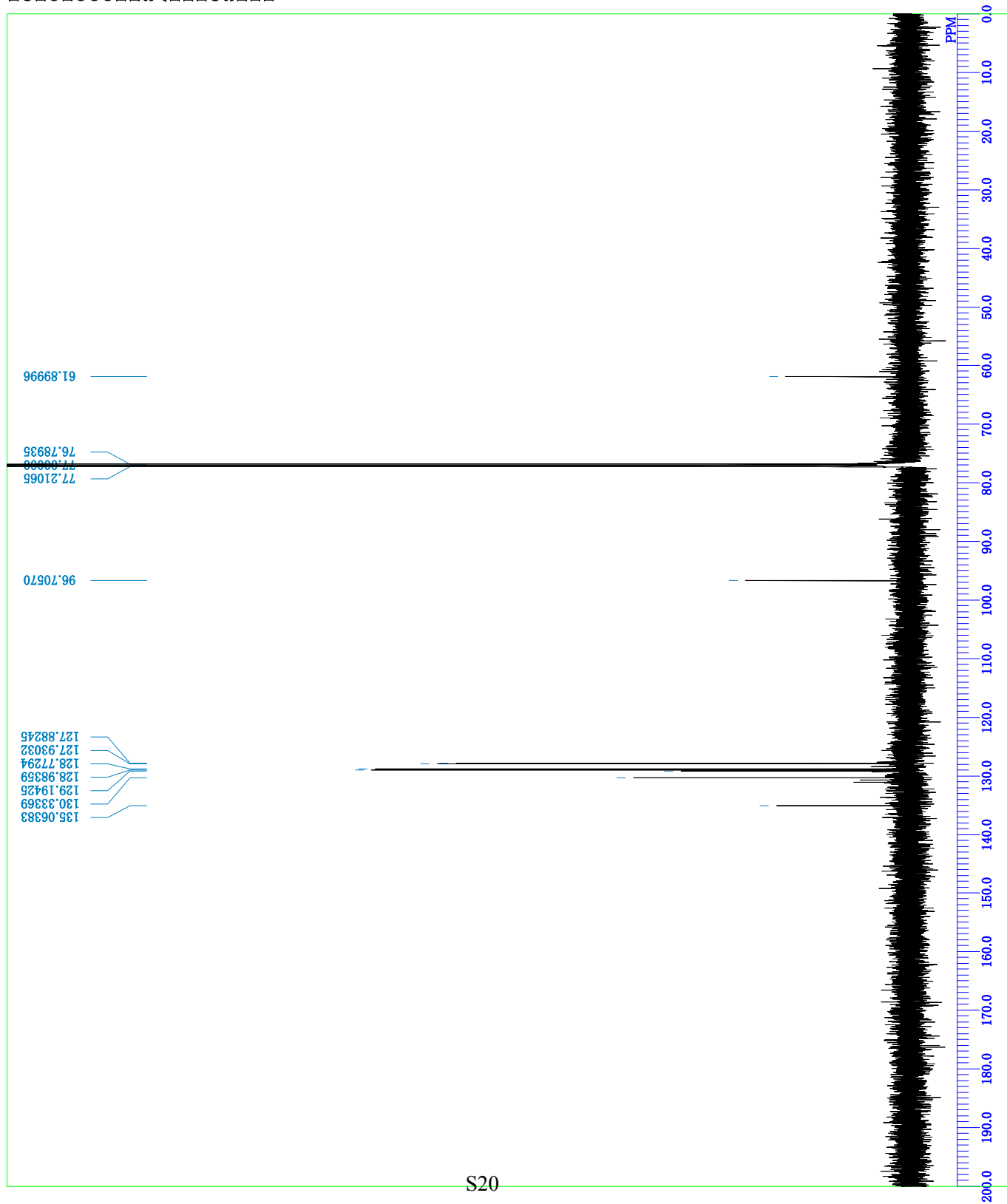


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COMINT 22-02-2010 20:34:50
DATIM 1H
OBNUC single pulse ex2
EXMOD 600.17 MHz
OBFRQ 5.30 KHz
OBSETT 5.47 Hz
OBFIN 13107
POINT 9008.87 Hz
FREQU 16
SCANS 1.4549 sec
ACQTM 2.0000 sec
PD 6.50 usec
PW1 1H
IRNUC 20.3 c
CTEMP CDCL3
SLVNT 0.00 ppm
EXREF BF 0.25 Hz
RGAIN 46



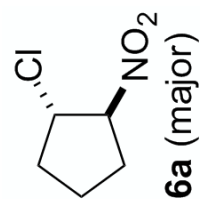
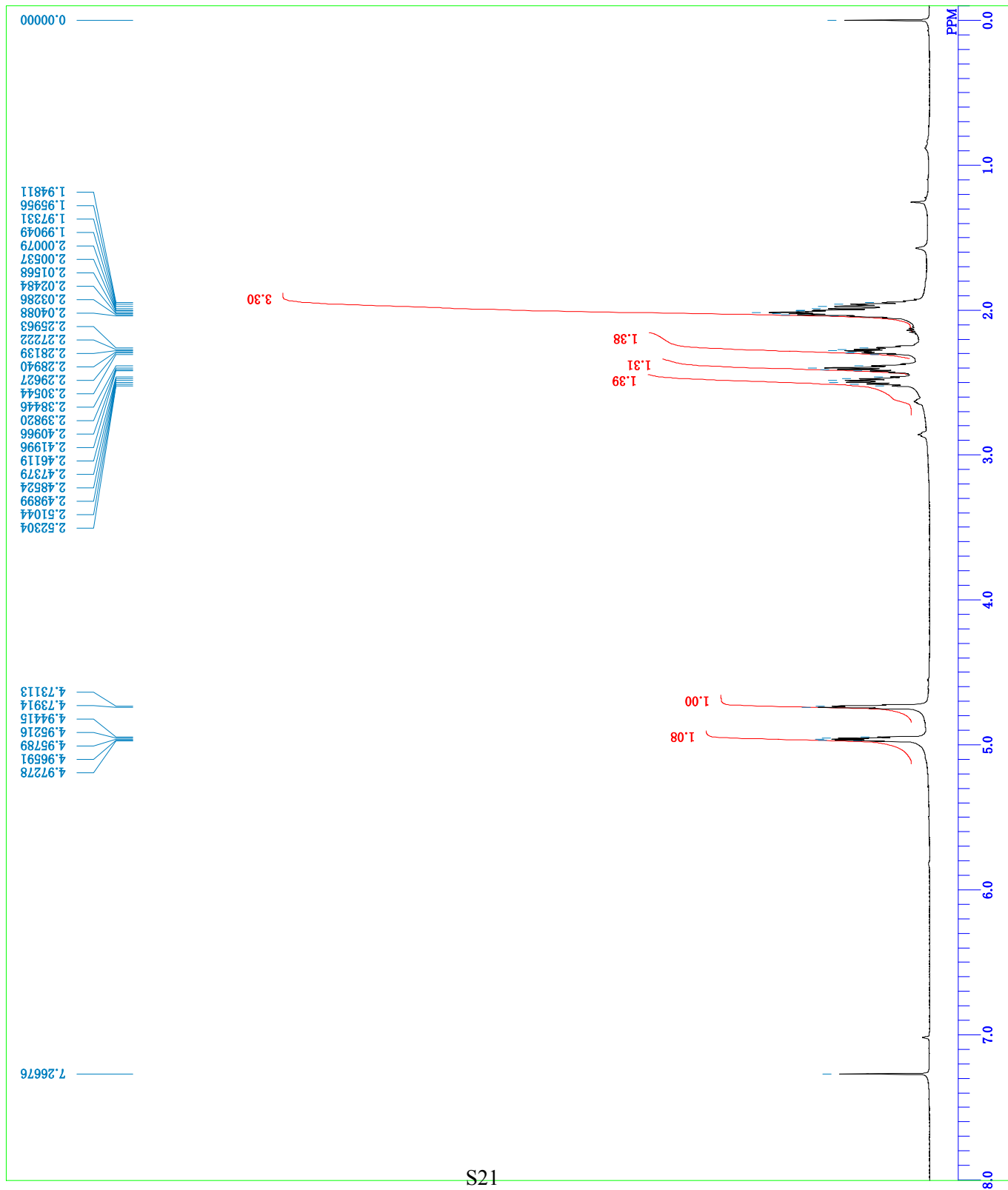
4f-C.als
100213
13-02-2010 16:28:29
13C
single_pulse_dec
150.92 MHz
8.52 KHz
1.74 Hz
20970
30302.11 Hz
514
0.6921 sec
1.2000 sec
4.00 usec
1H 19.8 c
CDCL3
77.00 ppm
0.12 Hz
56
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



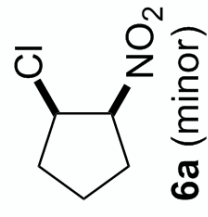
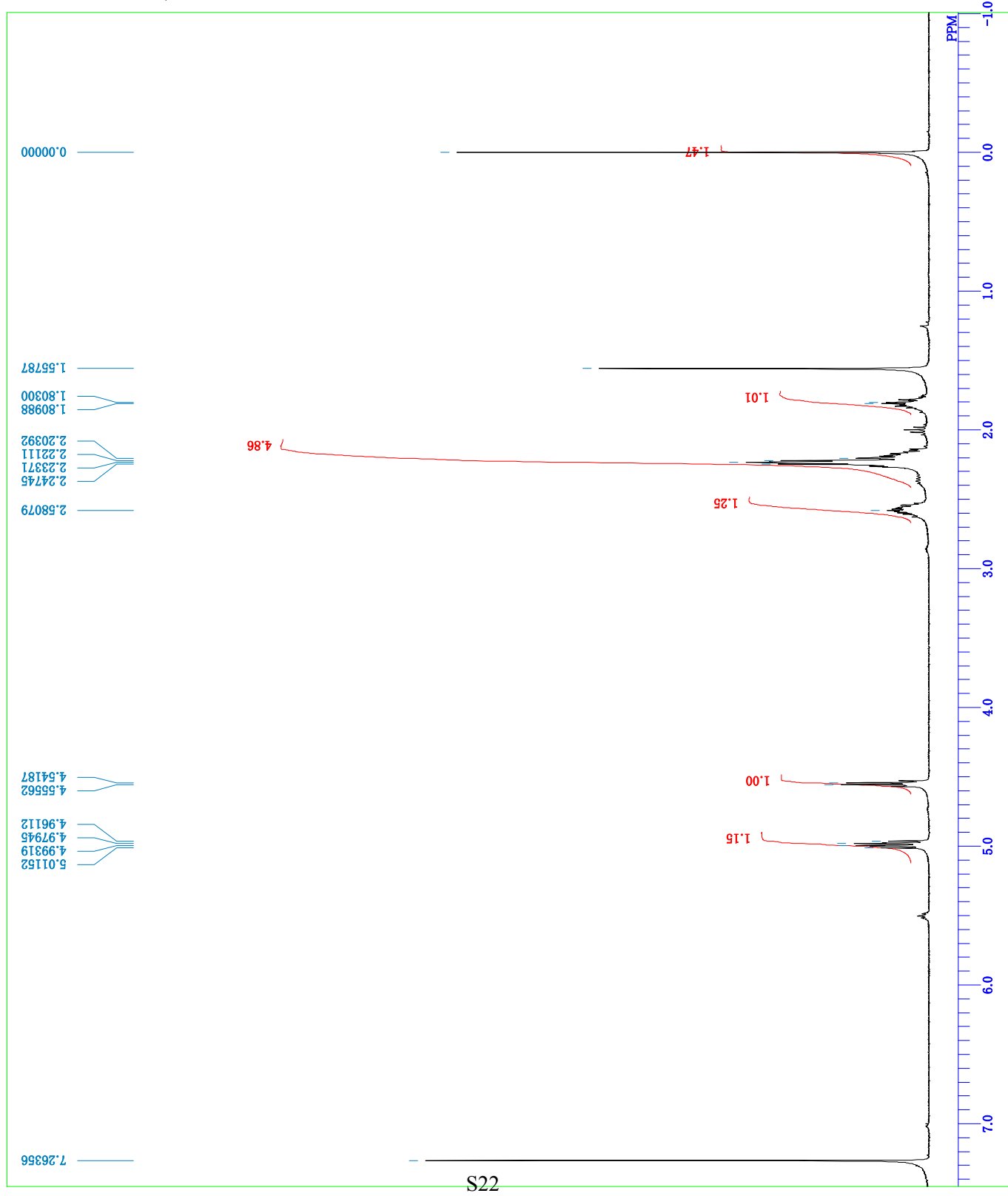
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 12-01-2010 16:33:11
 1H
 single pulse, ex2
 600.17 MHz
 5.30 KHz
 5.47 Hz
 10485
 7206.99 Hz
 16
 1.4549 sec
 2.0000 sec
 5.40 usec
 1H
 18.4 c
 CDCl₃
 0.00 ppm
 0.25 Hz
 42
 RGAIN

DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN



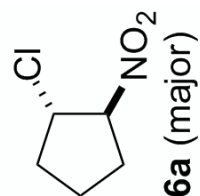
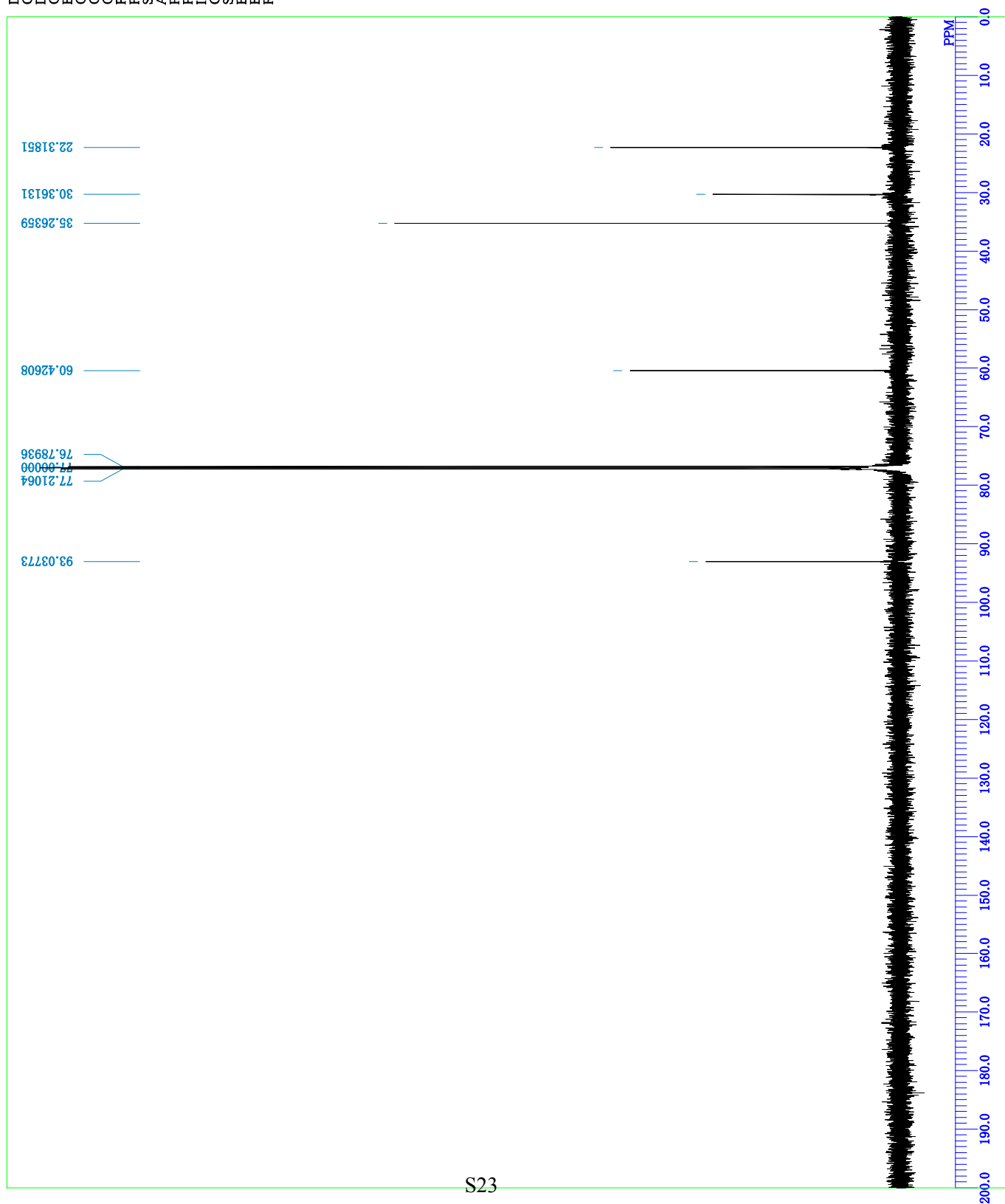
6a-minor-1H.als
100219
19-02-2010 10:29:55
1H
single_pulse.ex2
399.78 MHz
4.19 KHz
7.29 Hz
13107
6002.31 Hz
18
2.1837 sec
2.0000 sec
4.75 usec
1H 19.0 c
CDCl3
0.00 ppm
0.12 Hz
50
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSETT
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



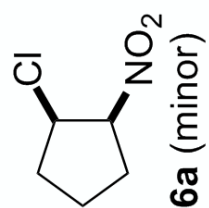
6a-major-Cals
100112
12-01-2010 16:42:47
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
259
0.6921 sec
1.2000 sec
2.77 usec
1H 19.0 c
CDCL3
77.00 ppm
0.25 Hz
54
RGAIN

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



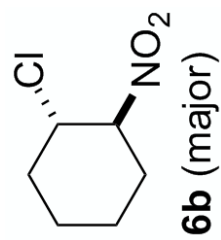
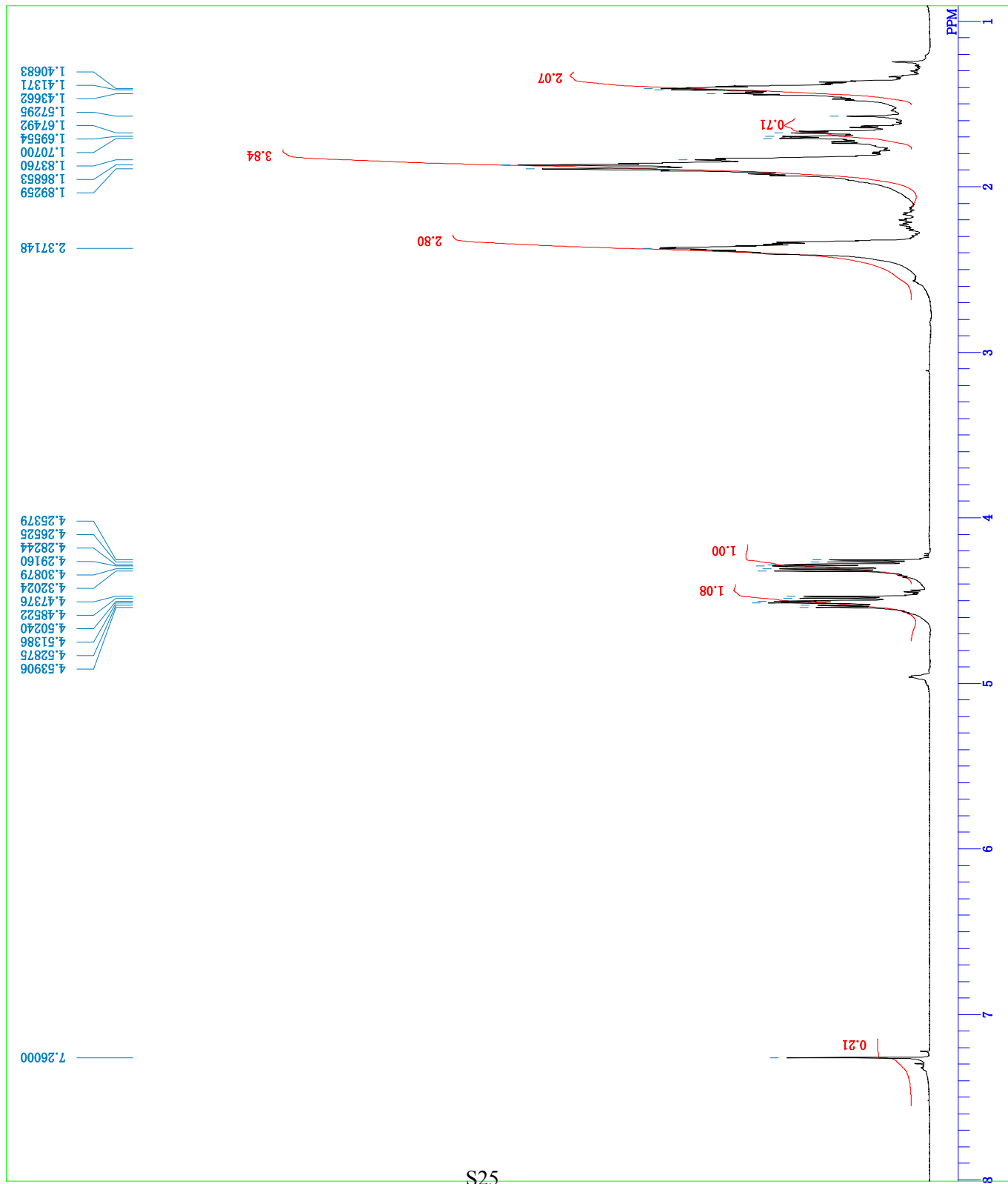
6a-minor-C.als
100220
20-02-2010 10:16:43
13C
single pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.24 Hz
1000
1.0433 sec
1.2000 sec
2.87 usec
1H 19.8 c
CDCL3
77.00 ppm
0.12 Hz
60
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



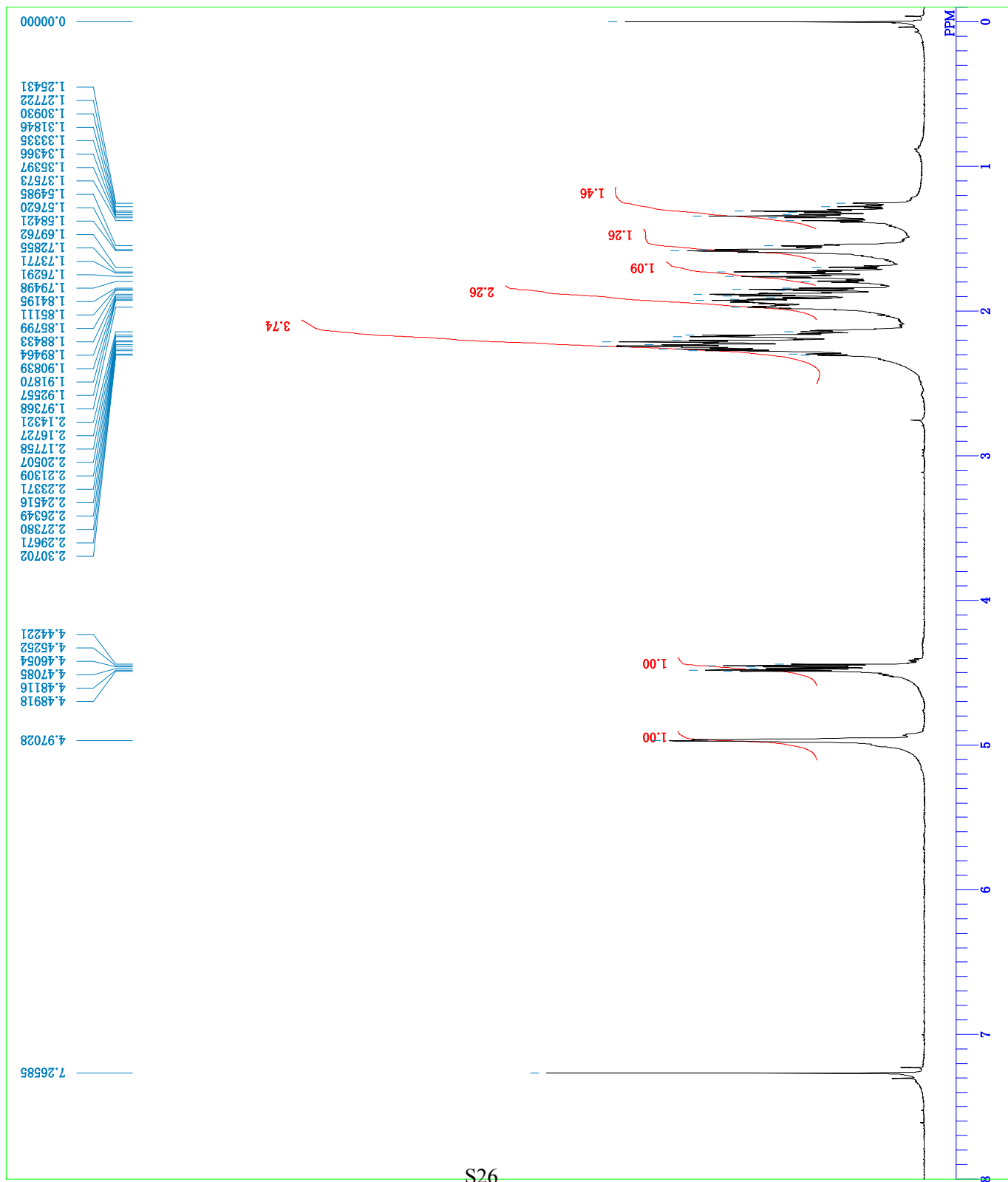
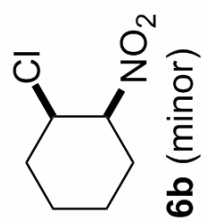
6b-major-1H.als
 091216
 16-12-2009 22:09:03
 1H
 single pulse, ex2
 399.78 MHz
 4.19 KHz
 7.29 Hz
 8387
 3841.36 Hz
 16
 2.1837 sec
 2.0000 sec
 4.75 usec
 1H
 19.8 c
 CDCl₃
 7.26 ppm
 0.16 Hz
 34
 RGAIN

DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN



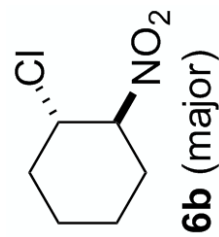
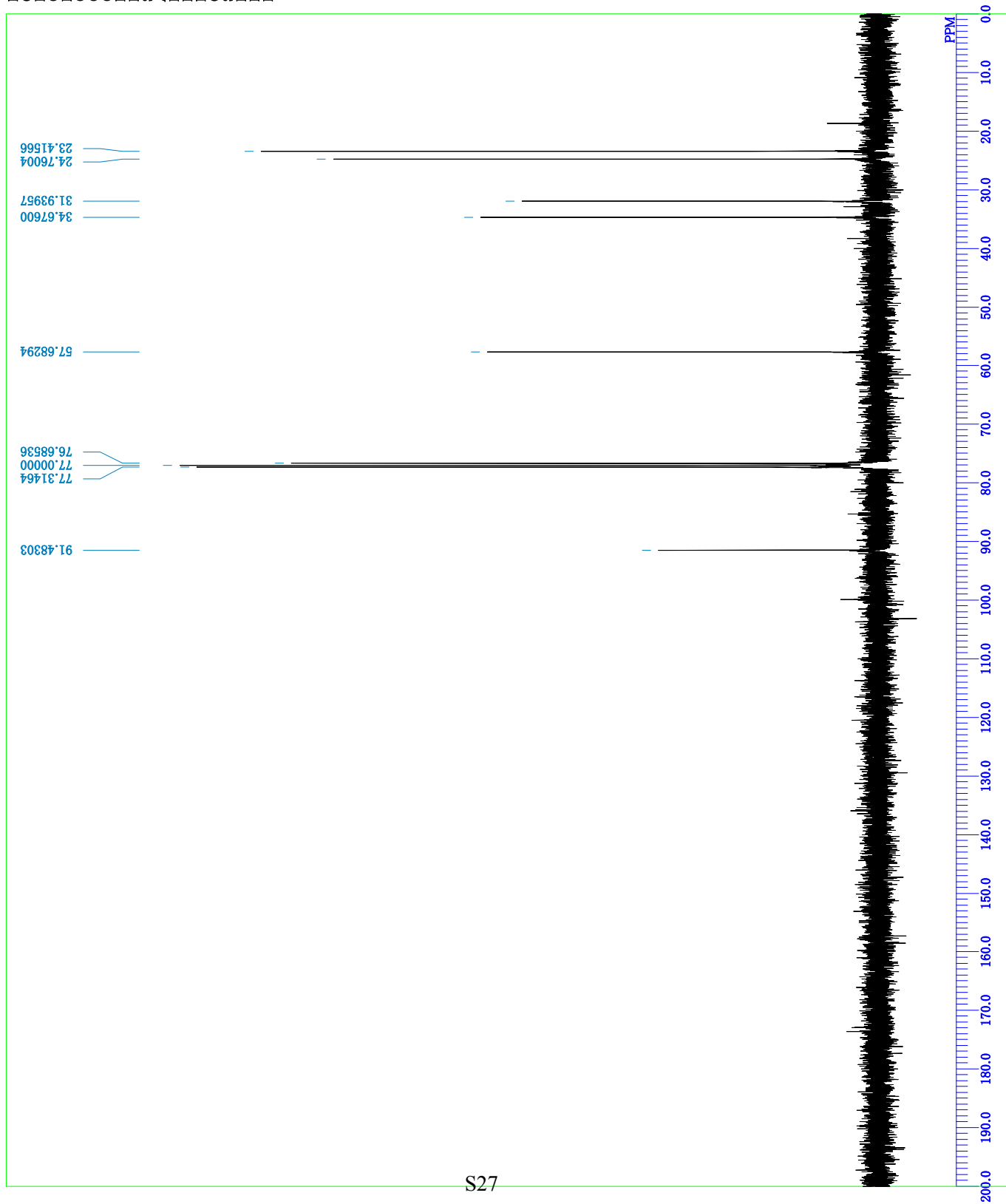
6b-minor-1H.as
 091216
 16-12-2009 22:26:04
 1H
 single pulse, ex2
 399.78 MHz
 4.19 KHz
 7.29 Hz
 13107
 POINT
 6002.31 Hz
 16
 SCANS
 2.1837 sec
 2.0000 sec
 PD
 4.75 usec
 1H
 19.8 c
 CDCL3
 0.00 ppm
 0.16 Hz
 BF
 40
 RGAIN

DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

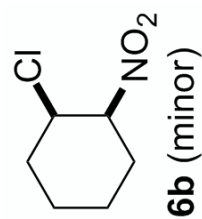
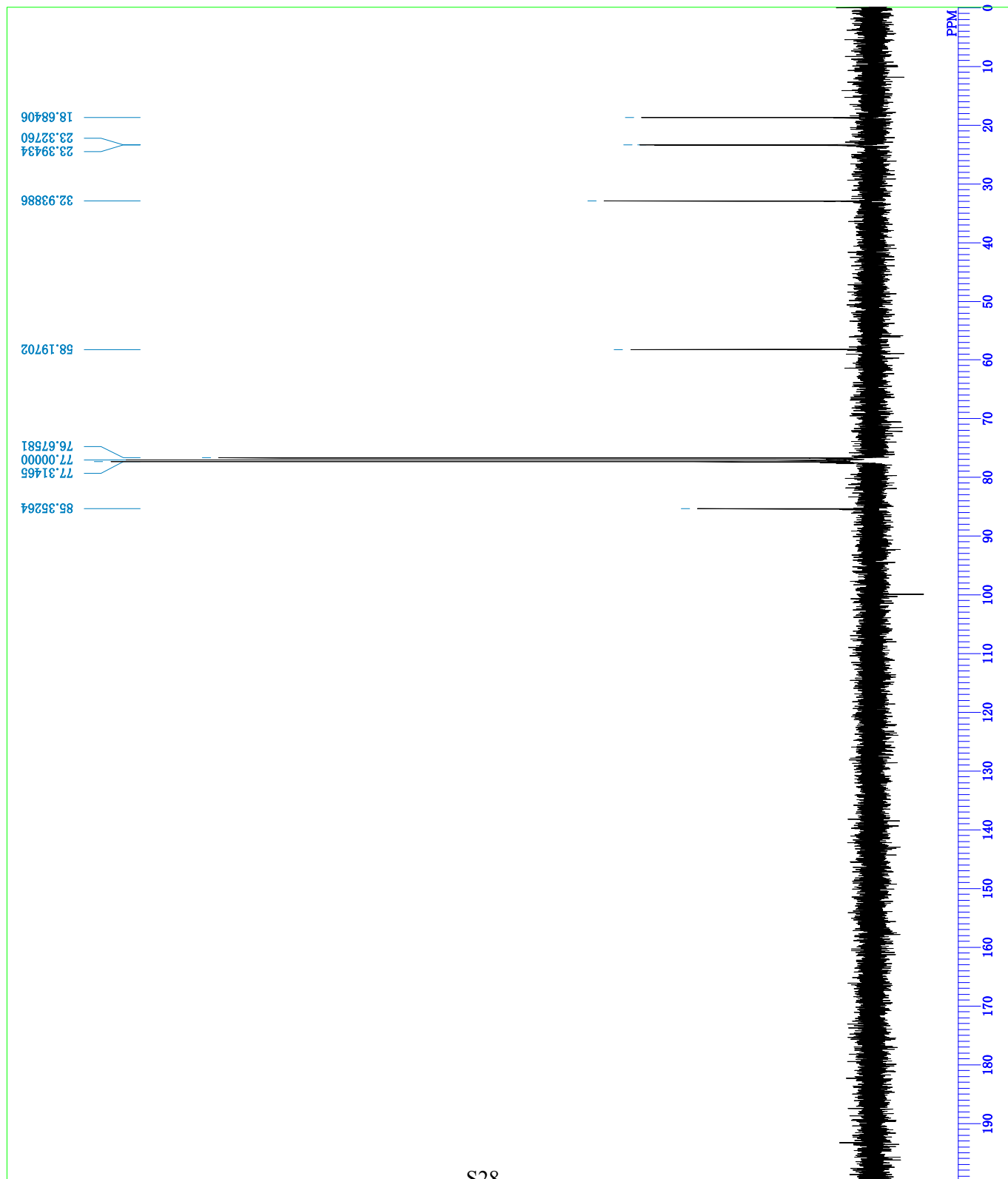


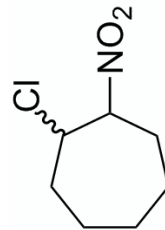
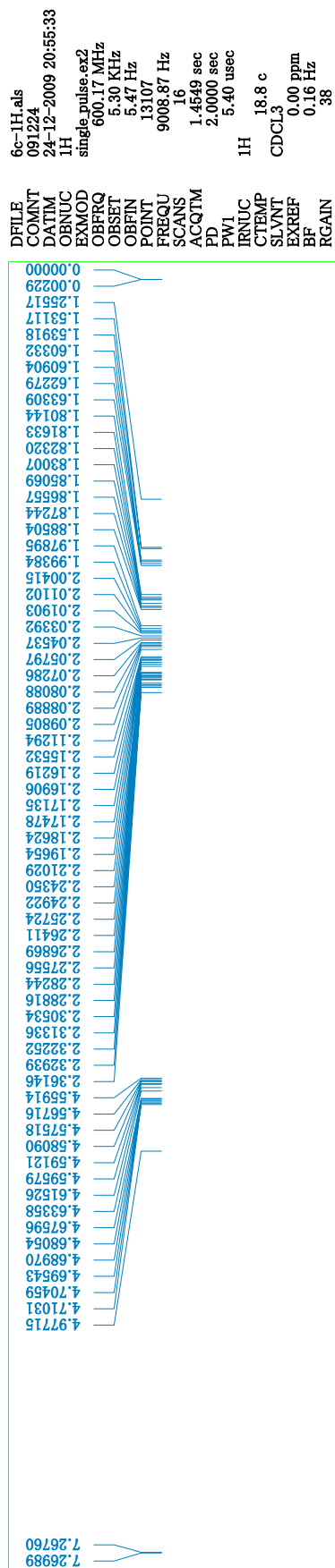
6-1-C.jdf
091216
16-12-2009 22:19:17
13C
single_pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
32768
31407.03 Hz
258
1.0433 sec
1.2000 sec
2.87 usec
1H
20.1 c
CDCL3
77.00 ppm
0.25 Hz
60
RGAIN

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



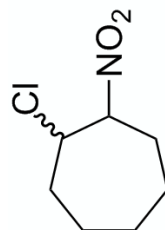
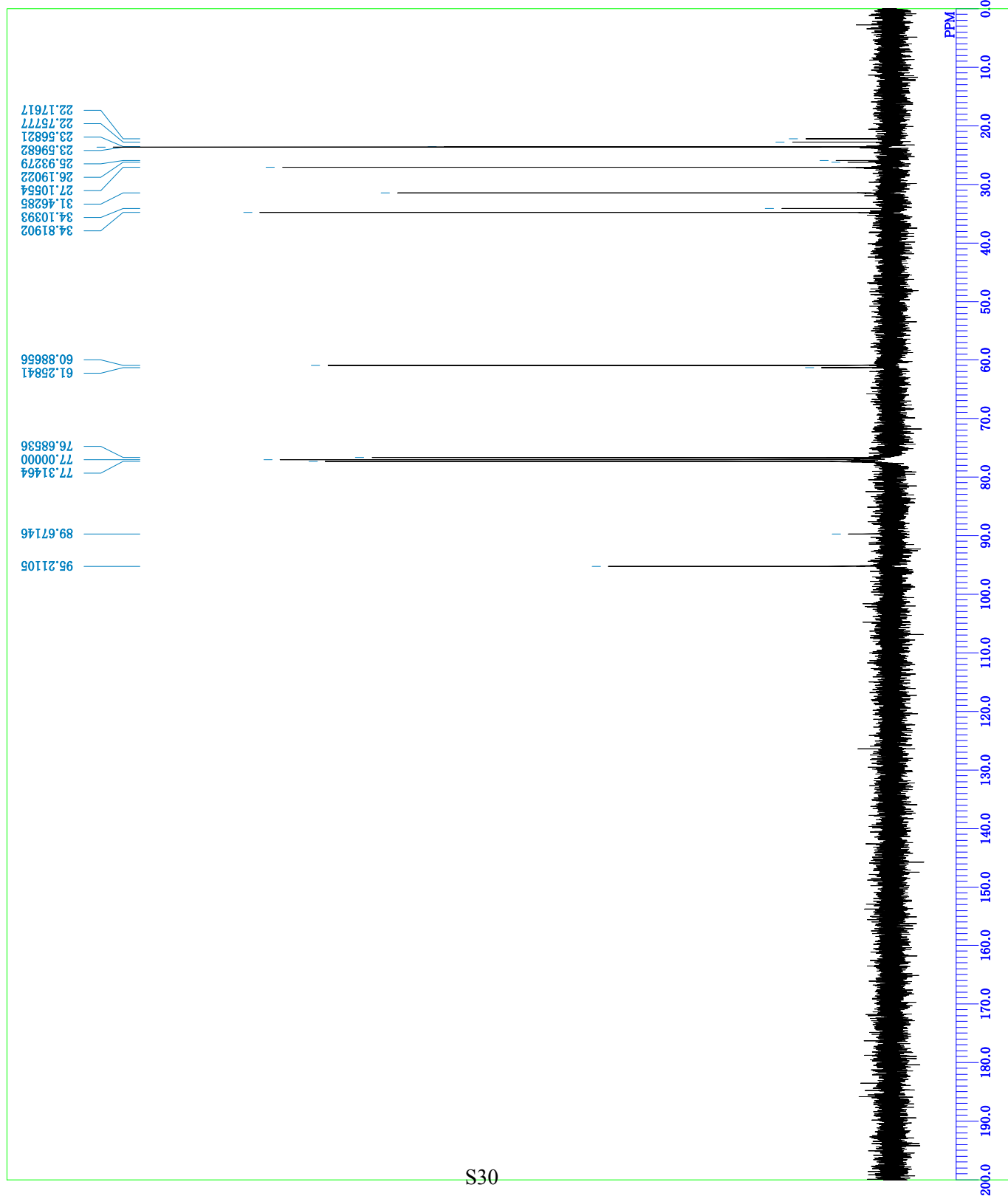
6b-minor-Cals
091216
16-12-2009 22:36:17
13C
single_pulse_dec
EXMOD 100.53 MHz
OBFRQ 5.35 KHz
OBSET 5.86 Hz
POINT 20970
FREQ 20099.89 Hz
SCANS 258
ACQTM 1.0433 sec
PD 1.2000 sec
PW1 2.87 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.16 Hz
RGAIN 60





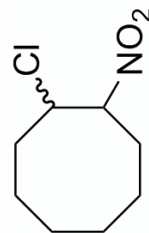
6c (*trans:cis*, 87:13)

6c-Cals
 091221
 21-12-2009 21:19:53
 13C
 single pulse dec
 100.53 MHz
 5.35 KHz
 5.86 Hz
 26214
 25125.24 Hz
 262
 1.0433 sec
 1.2000 sec
 2.87 usec
 1H 17.9 c
 CDCL3
 77.00 ppm
 0.00 Hz
 60
 RGAIN

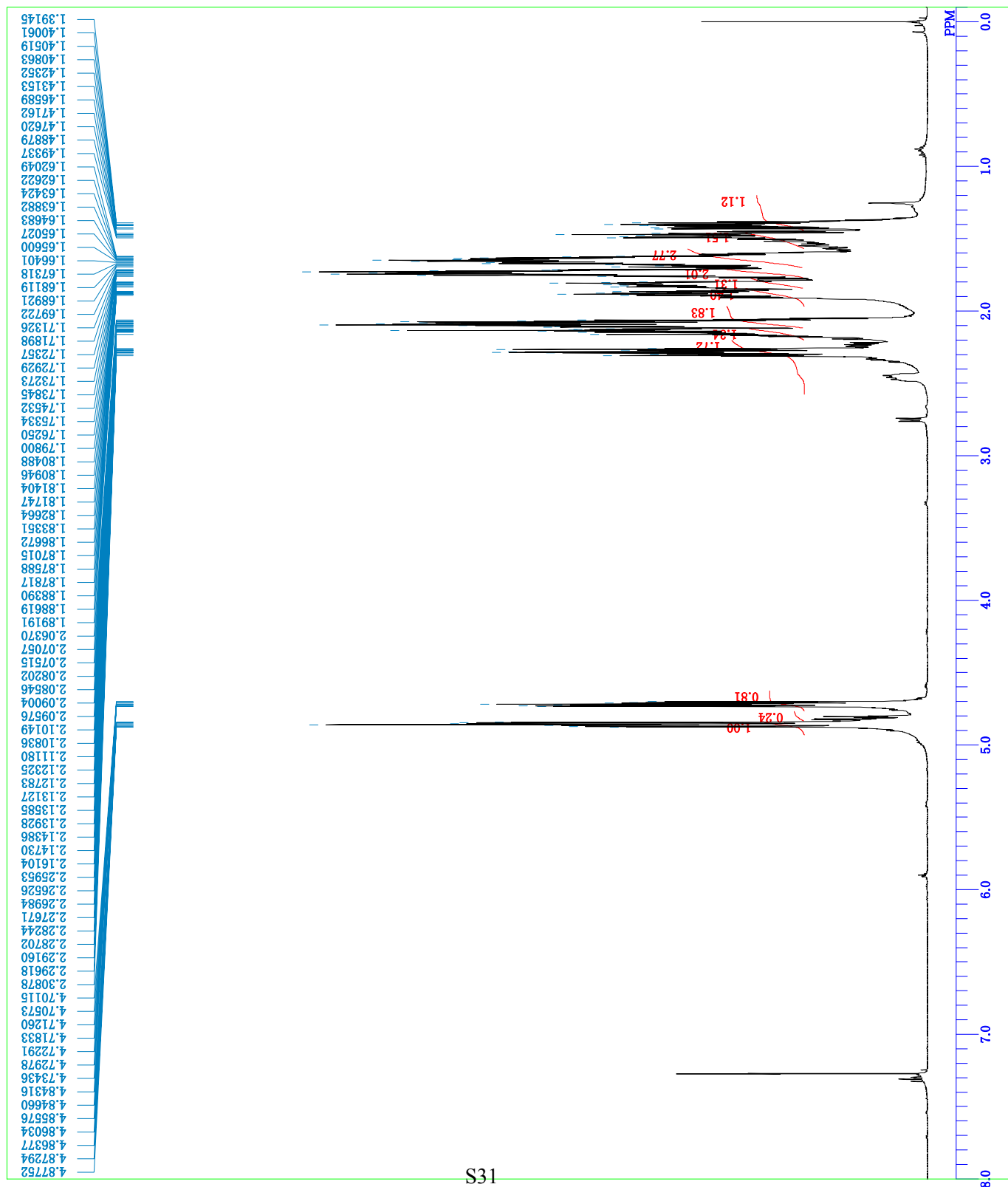


6c (trans:cis, 87:13)

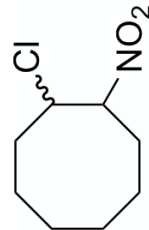
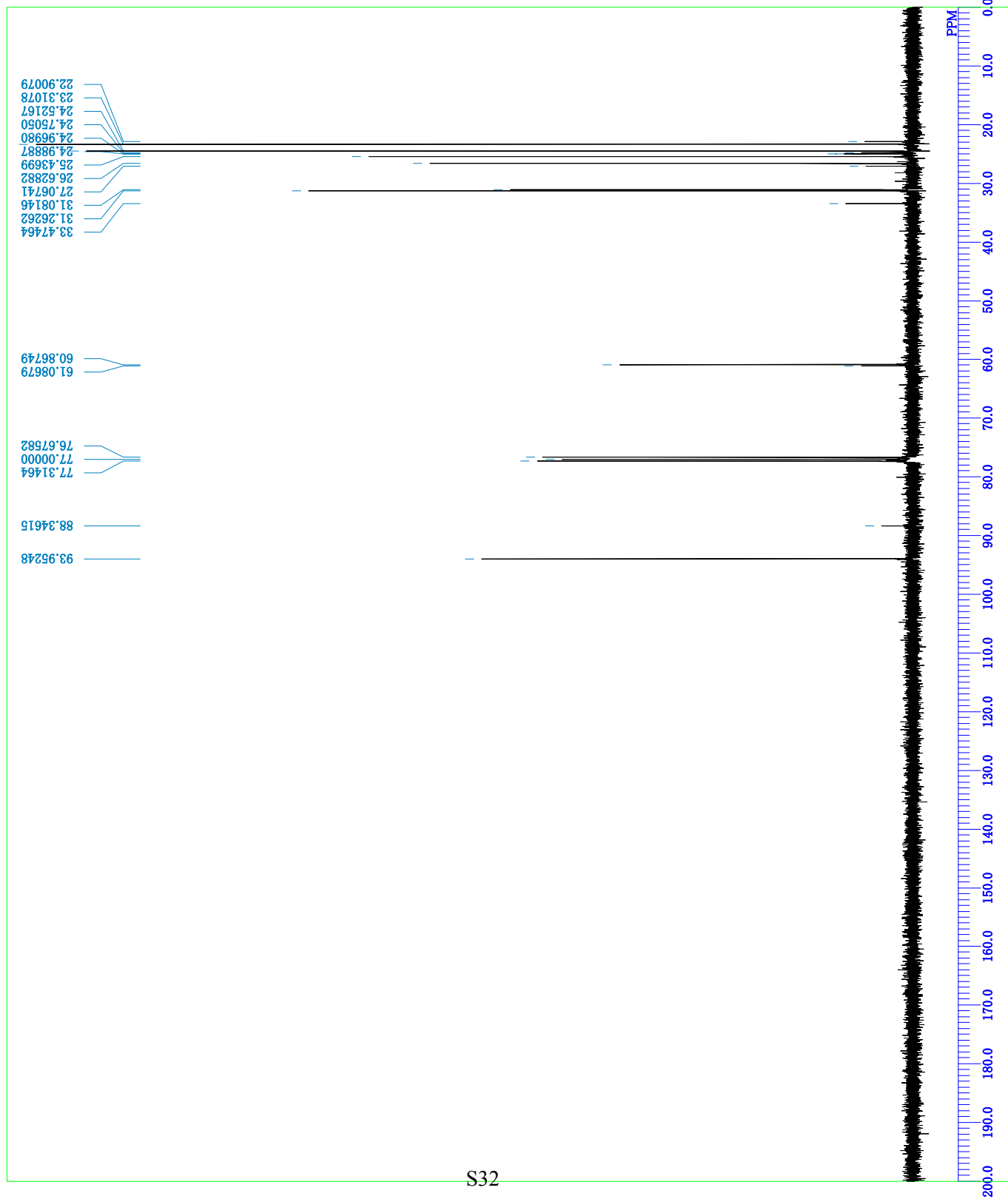
DFILE 6d-1H.als
 COMINT 100105
 DATIM 05-01-2010 17:24:41
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 600.17 MHz
 OBSET 5.30 KHz
 OBFIN 5.47 Hz
 POINT 13107
 FREQU 9008.87 Hz
 SCANS 16
 ACQTM 1.4549 sec
 PD 2.0000 sec
 PW1 5.40 usec
 IRNUC 1H
 CTEMP 17.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30



6d (*trans:cis*, 82:18)



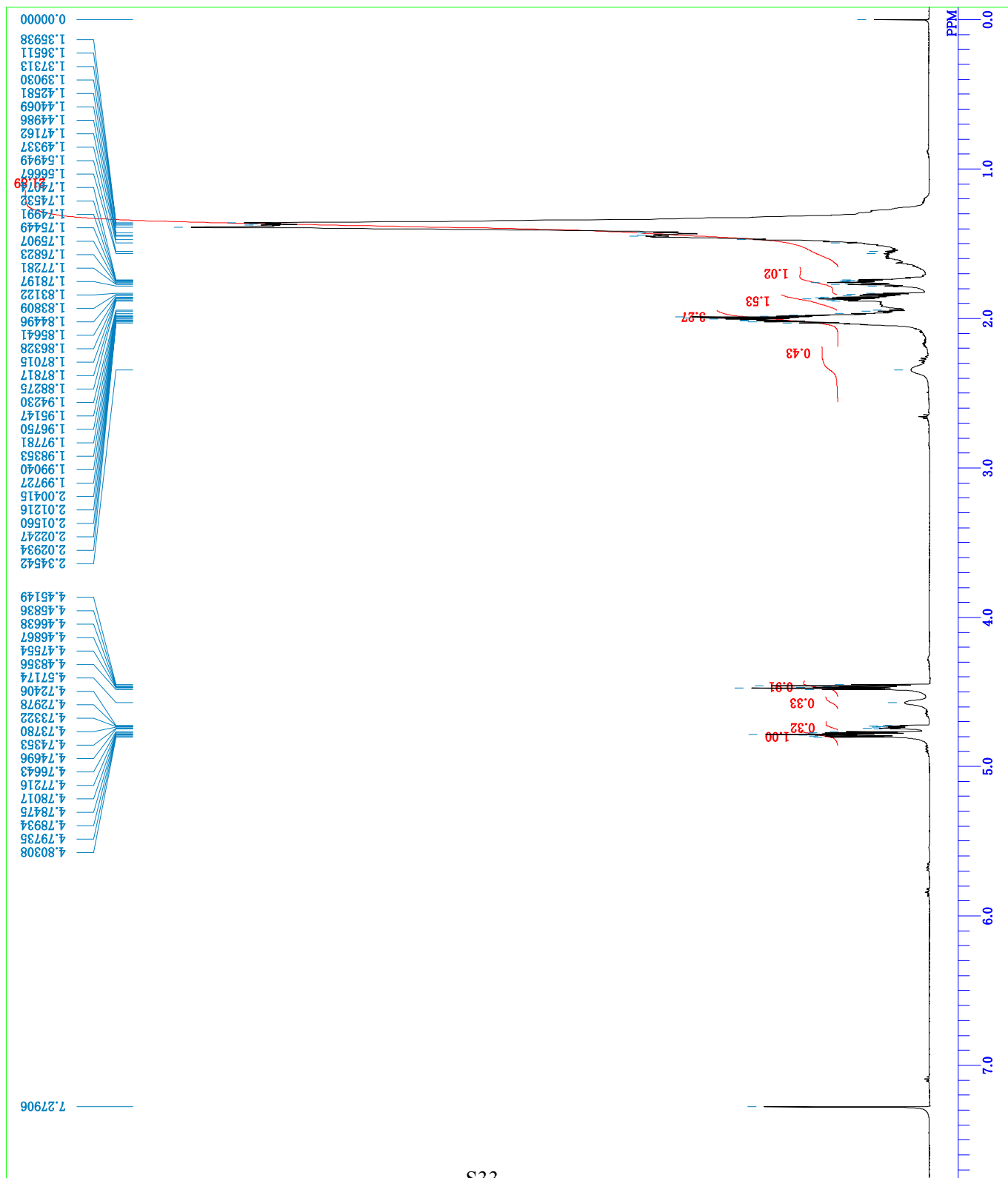
6d-C.als
 091221
 21-12-2009 21:38:36
 13C
 single pulse dec
 100.53 MHz
 5.35 KHz
 5.86 Hz
 26214
 25125.24 Hz
 290
 1.0433 sec
 1.2000 sec
 2.87 usec
 1H
 17.8 c
 CDCL3
 77.00 ppm
 0.00 Hz
 60
 RGAIN



6d (trans:cis, 82:18)

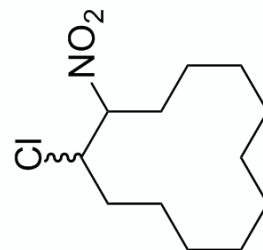
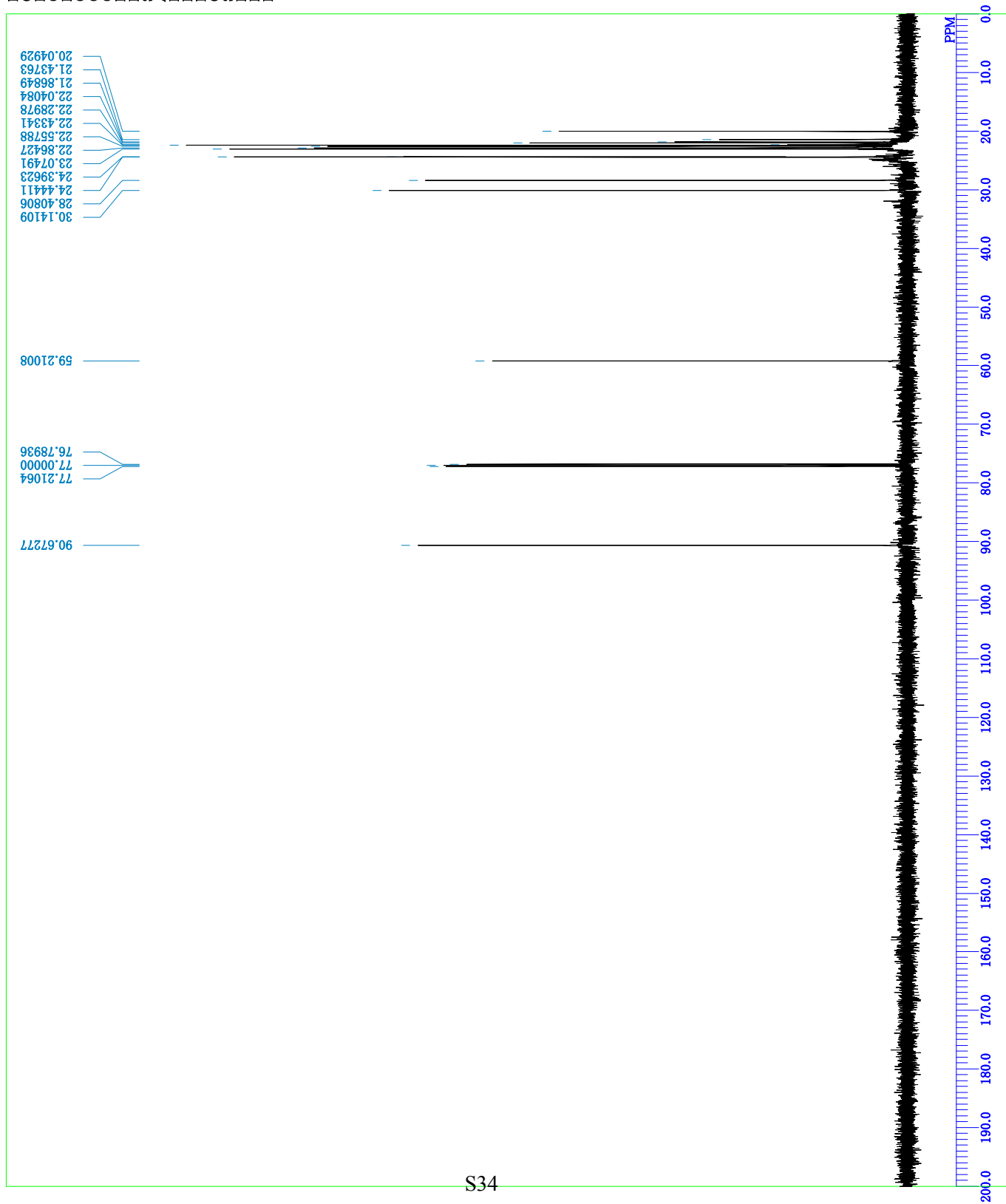
DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

6e-1H.als
 100226
 26-02-2010 22:08:04
 1H
 single pulse, ex2
 600.17 MHz
 5.30 KHz
 5.47 Hz
 13107
 9008.87 Hz
 16
 1.4549 sec
 2.0000 sec
 6.50 usec
 1H
 20.6 c
 CDCL3
 0.00 ppm
 0.12 Hz
 24



6e-C.als
100226
26-02-2010 22:51:23
13C
single_pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
162
0.6921 sec
1.2000 sec
4.00 usec
1H
21.3 c
CDCL3
77.00 ppm
0.12 Hz
56
RGAIN

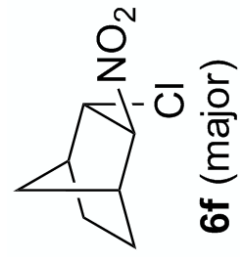
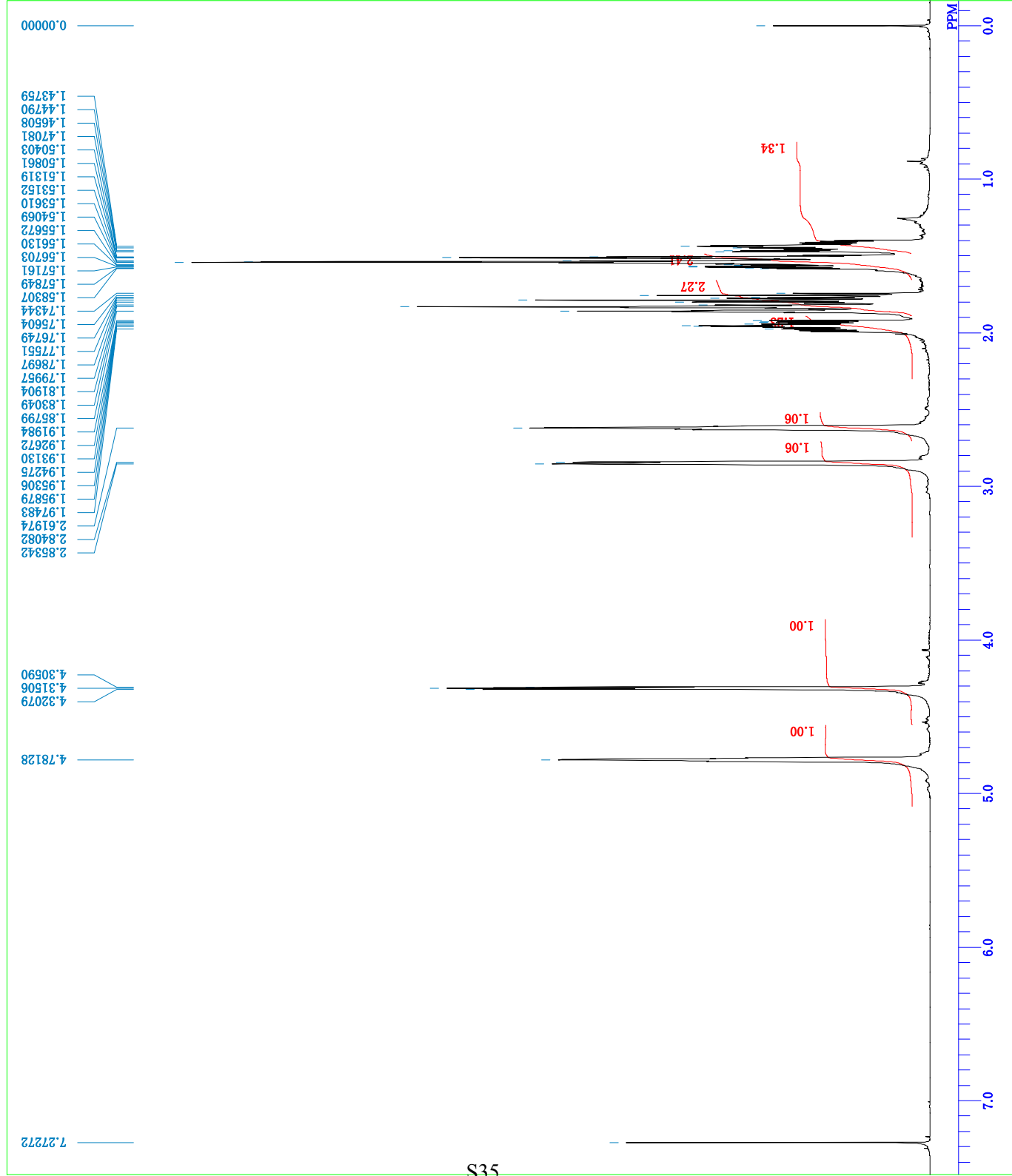
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFREQ
OBSETT
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



6e (trans:cis, 72:28)

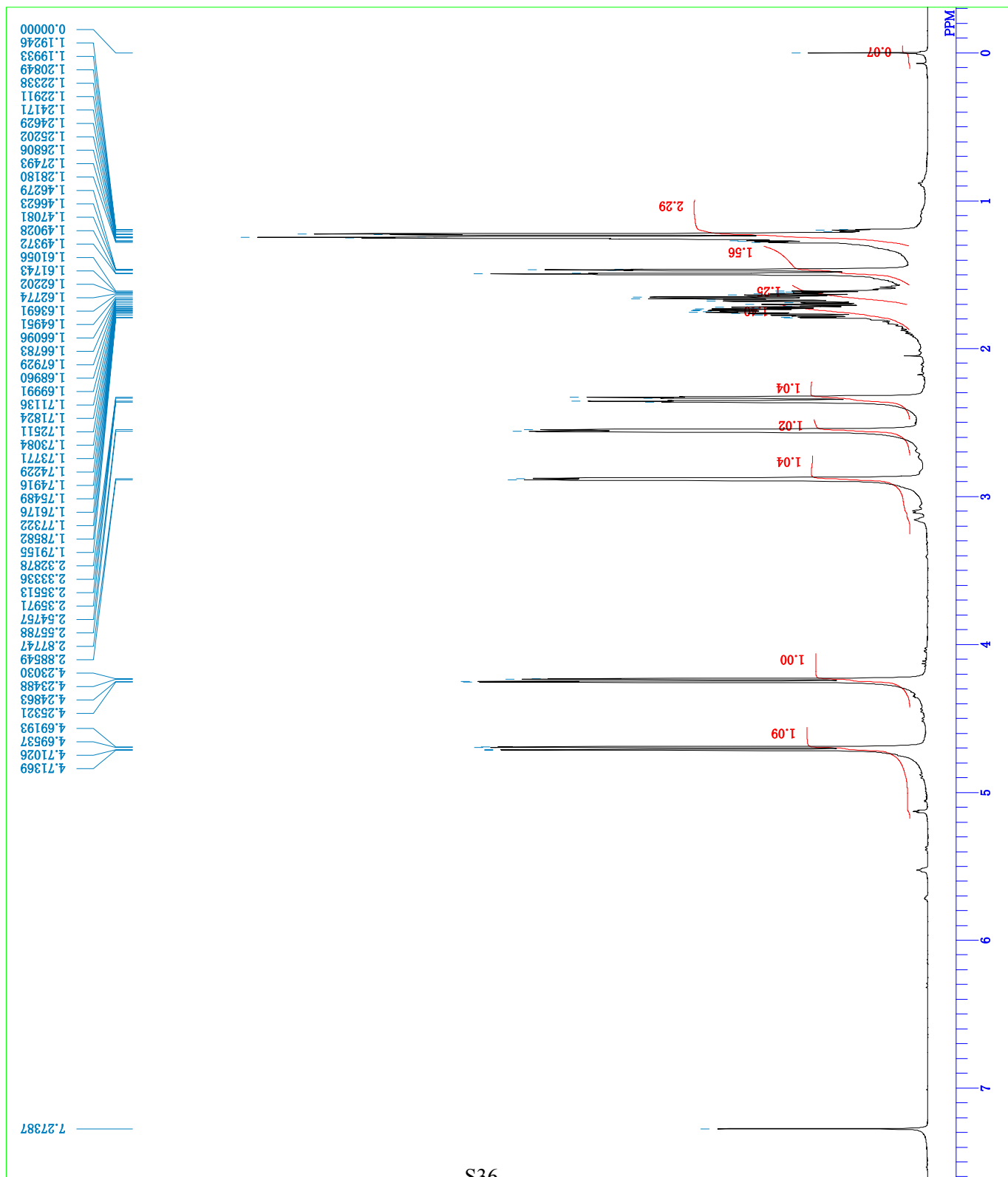
6f-major-1H.als
 100126
 26-01-2010 21:52:51
 1H
 single pulse, ex2
 399.78 MHz
 4.19 KHz
 7.29 Hz
 13107
 6002.31 Hz
 16
 2.1837 sec
 2.0000 sec
 4.75 usec
 1H
 19.3 c
 CDCL3
 0.00 ppm
 0.25 Hz
 30
 RGAIN

DFILE
 COMINT
 DATUM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN



DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

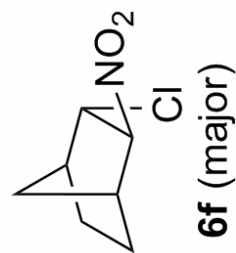
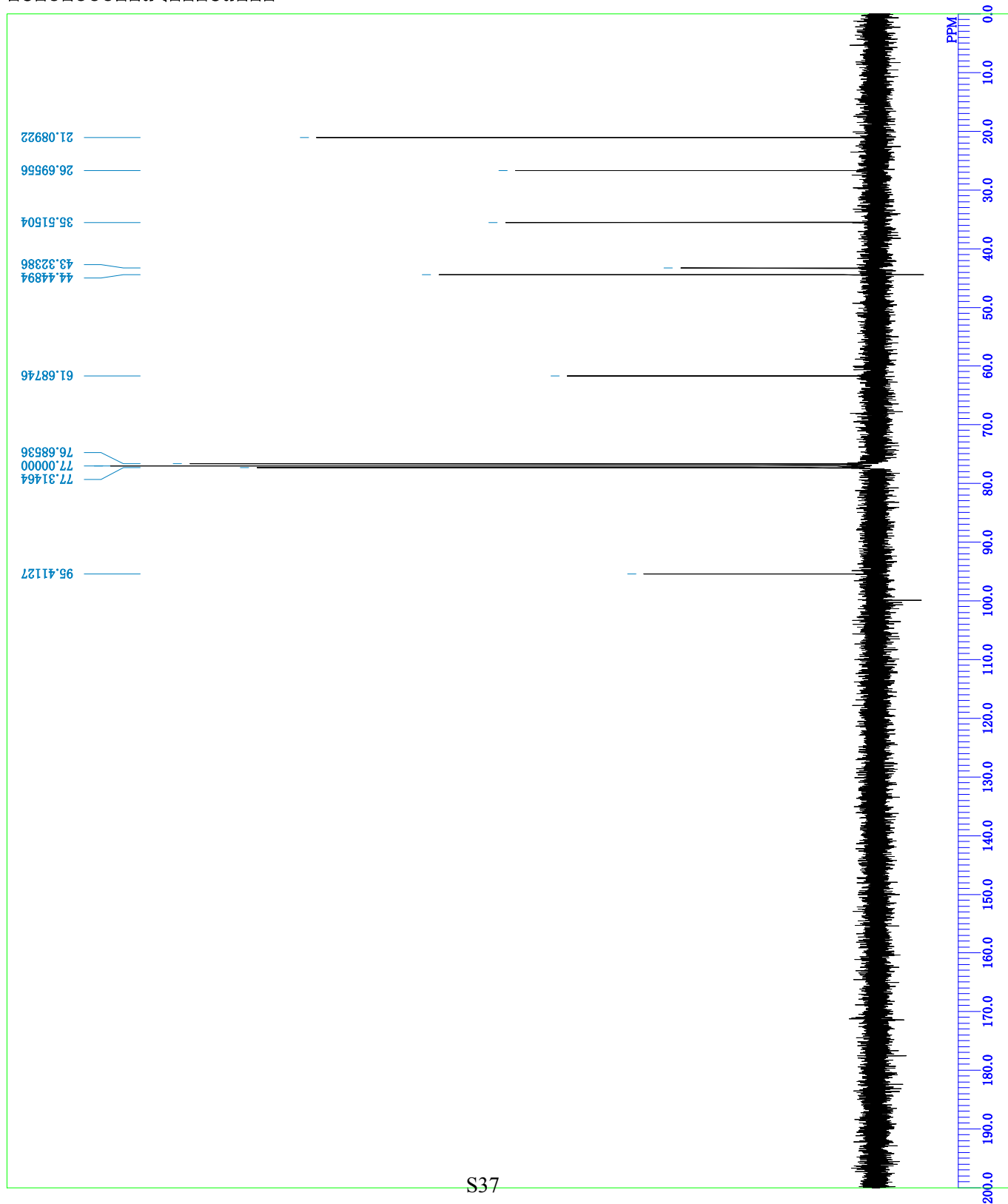
6f-minor-1H.als
 100119
 19-01-2010 21:46:03
 1H
 single pulse, ex2
 399.78 MHz
 4.19 KHz
 7.29 Hz
 13107
 6002.31 Hz
 16
 2.1837 sec
 2.0000 sec
 4.75 usec
 1H
 19.1 c
 CDCL3
 0.00 ppm
 0.25 Hz
 30



6f (minor)

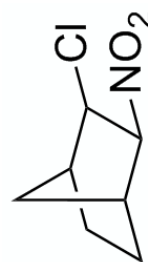
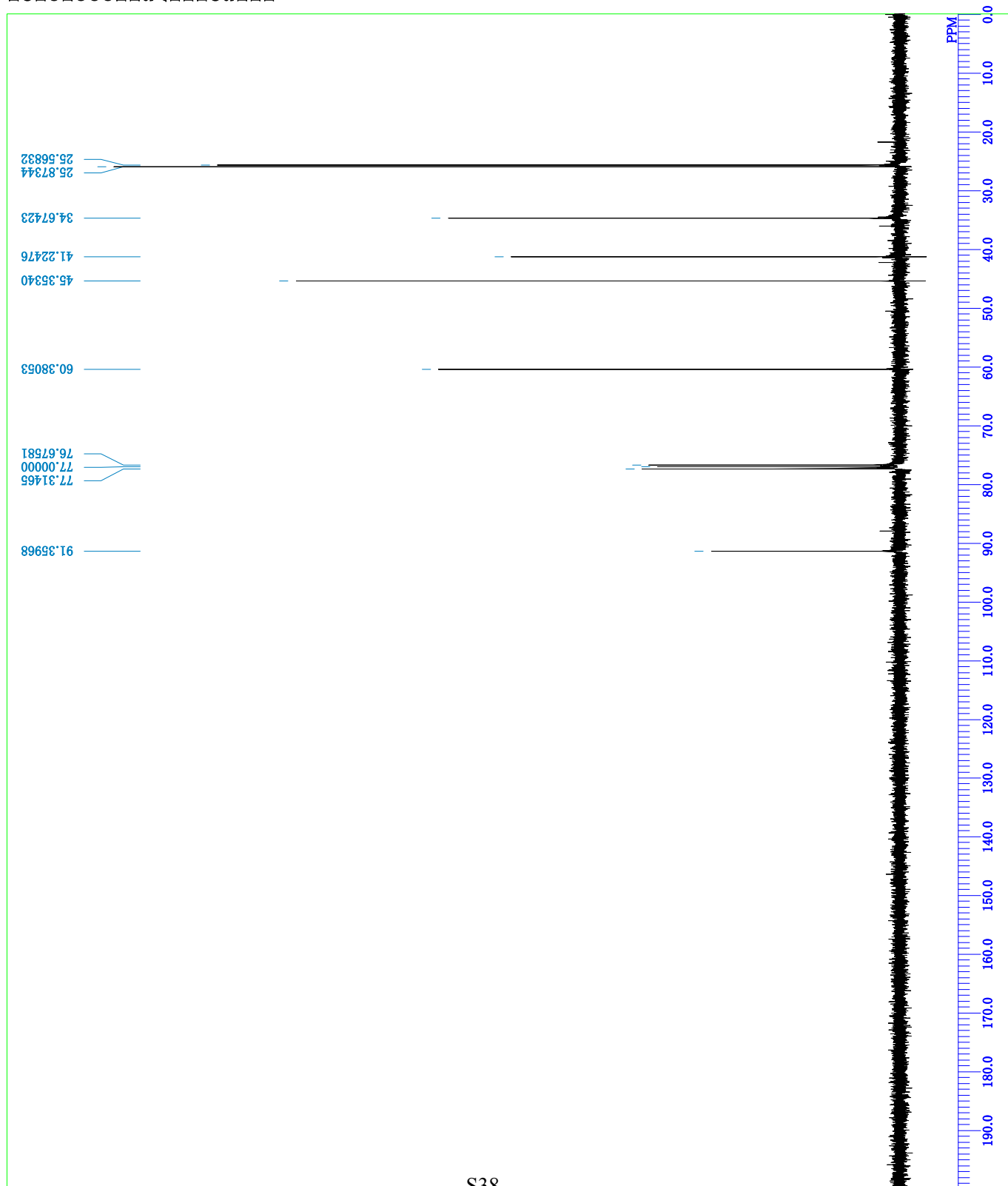
6f-major-C.als
100105
05-01-2010 21:35:41
13C
single pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
26214
258
25125.24 Hz
SCANS
1.0433 sec
1.2000 sec
PD
2.87 usec
PW1
1H 18.5 c
CDCL3
77.00 ppm
BF
0.00 Hz
60
RGAIN

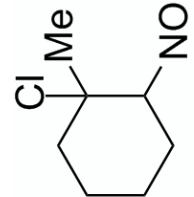
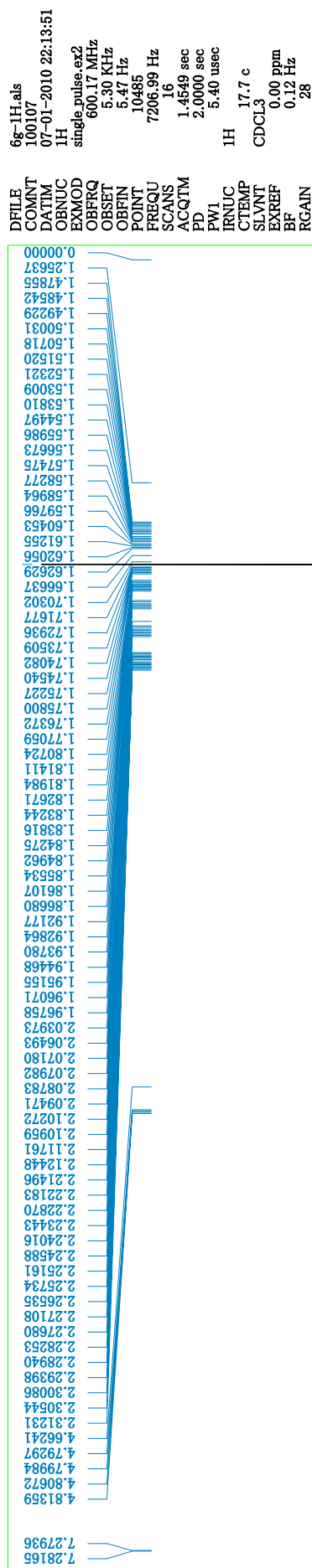
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



6f-minor-C.als
100105
05-01-2010 21:20:25
13C
single pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
20970
20099.89 Hz
169
1.0433 sec
1.2000 sec
2.87 usec
1H 18.4 c
CDCL3
77.00 ppm
0.00 Hz
60
RGAIN

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

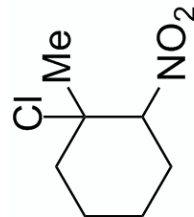
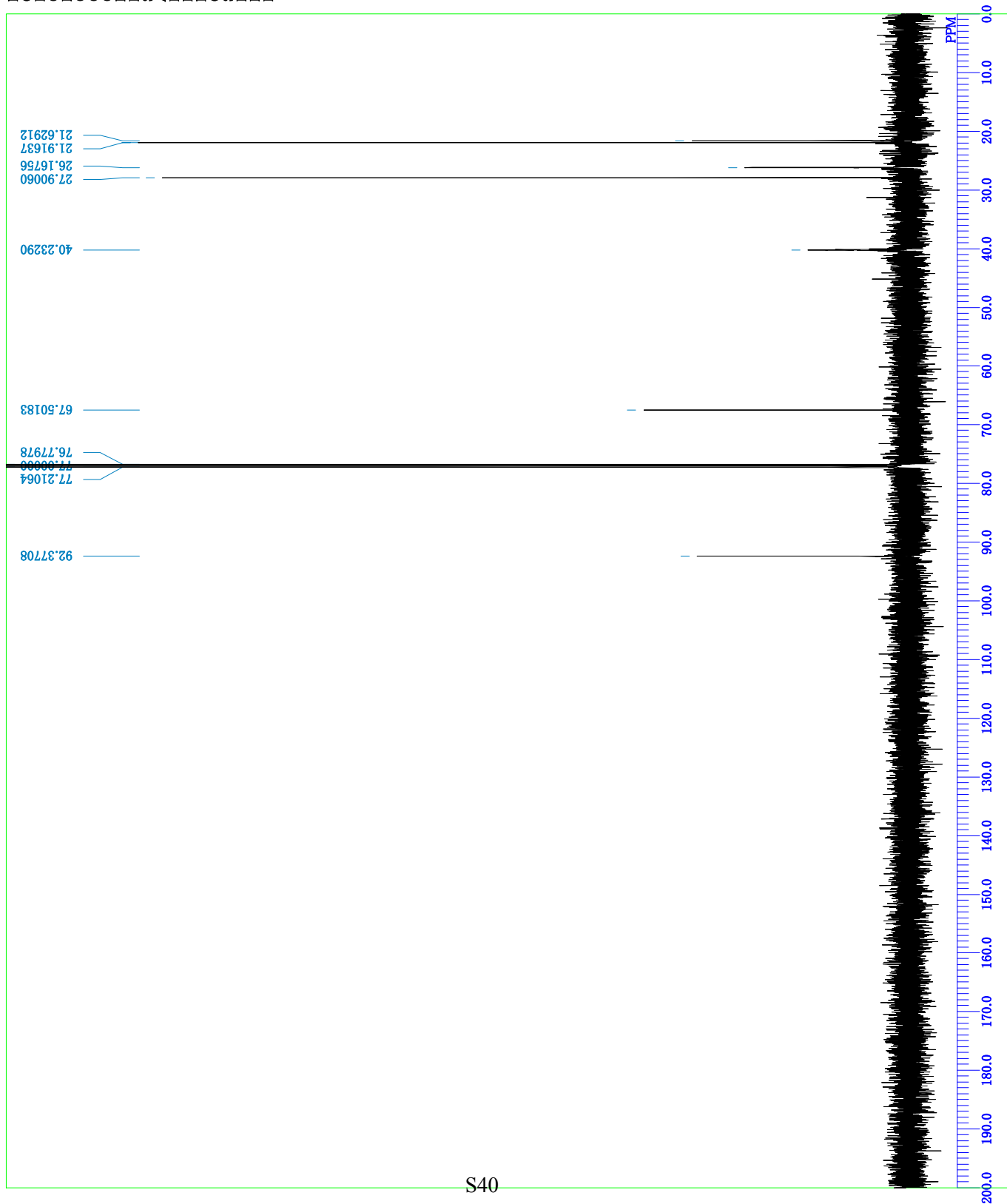
**6f (minor)**



6g (single isomer)

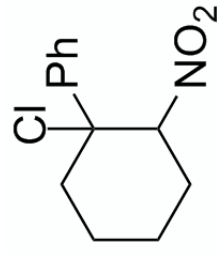
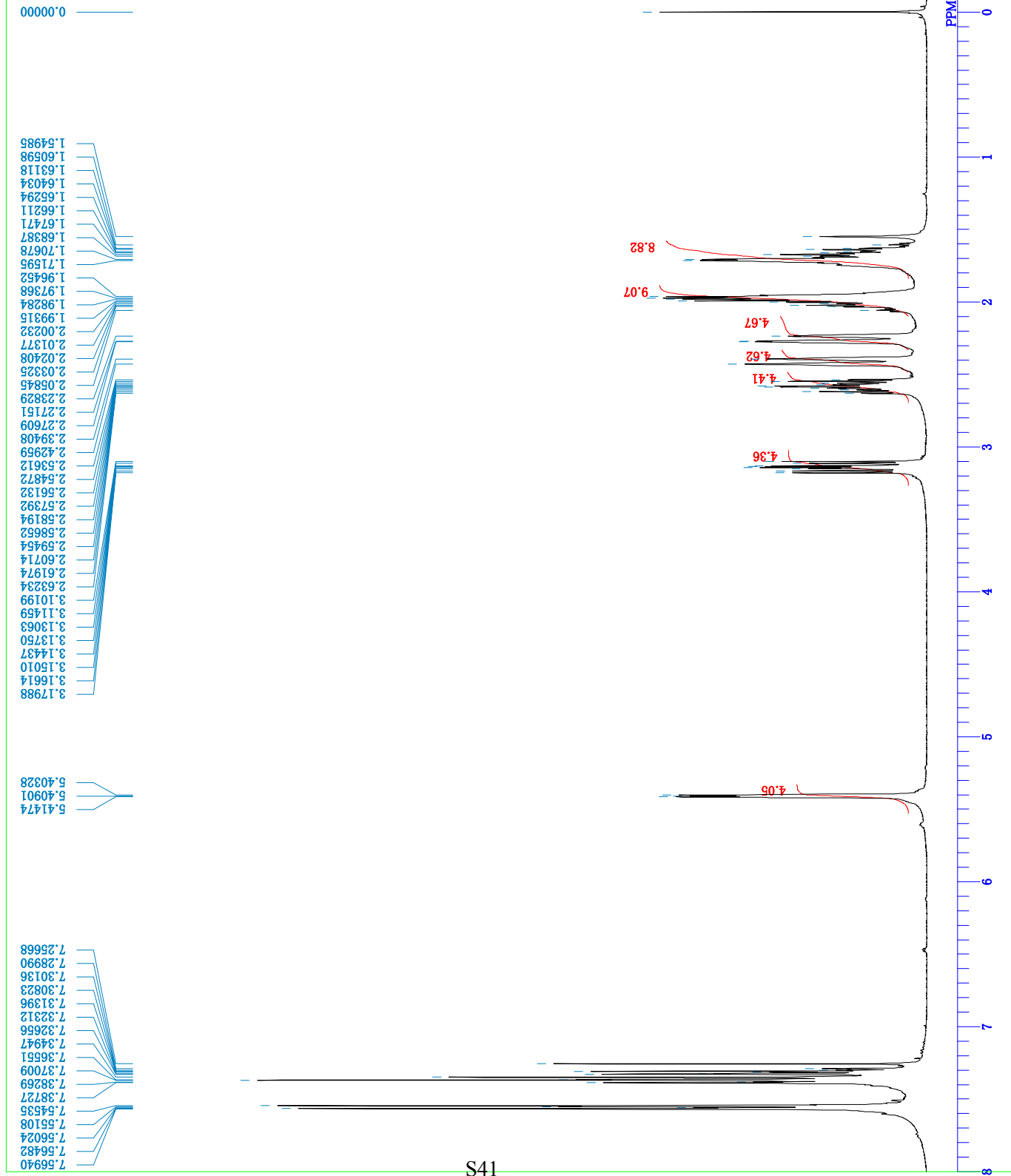
6g-C.as
100114
13-01-2010 21:11:41
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
258
0.6921 sec
1.2000 sec
2.77 usec
1H 17.4 c
CDCL3
77.00 ppm
0.25 Hz
54
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



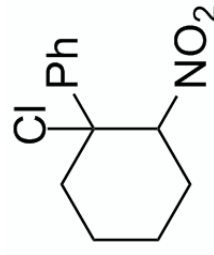
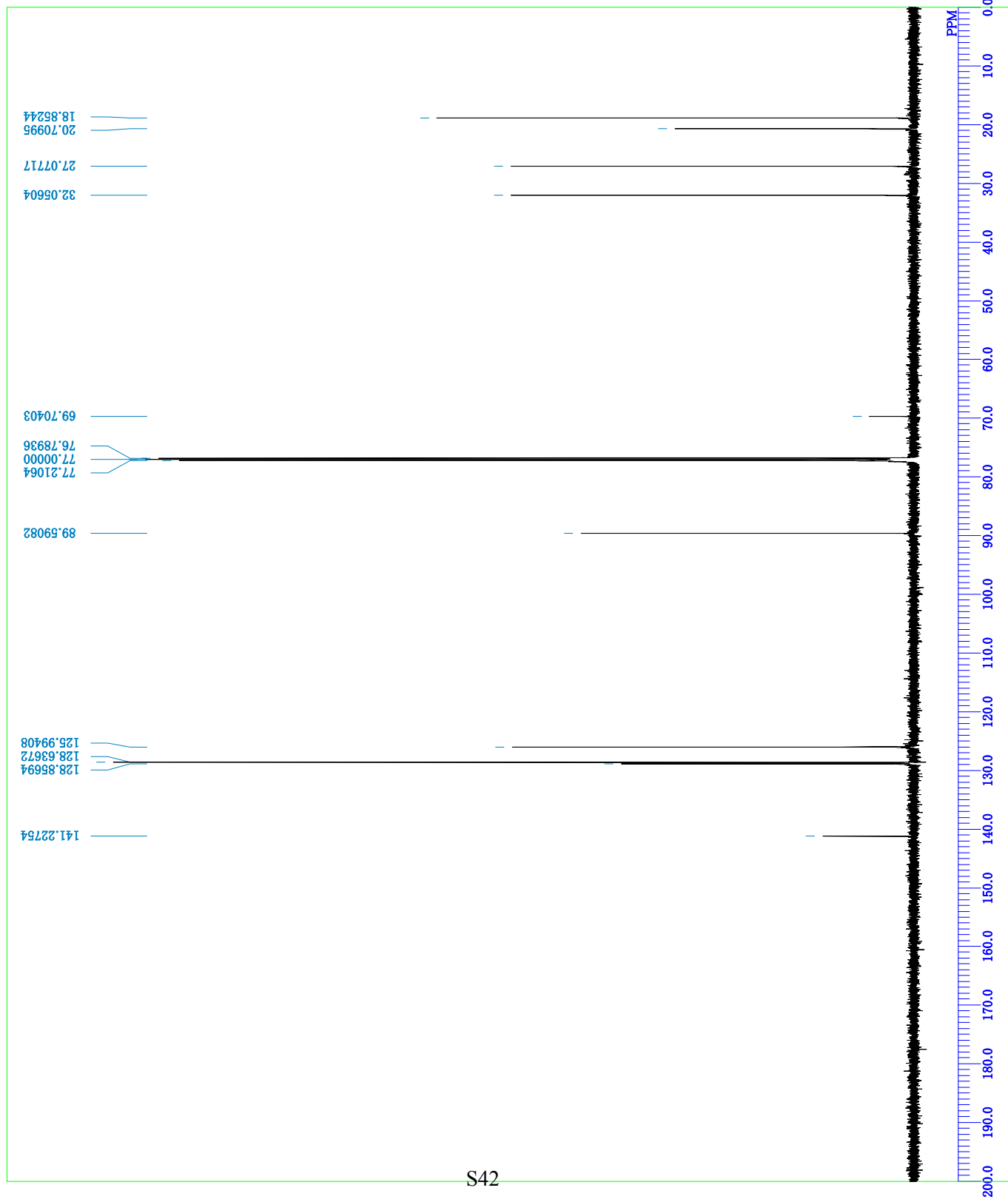
6g (single isomer)

DFILE 6h-1H.als
 COMINT 100125
 DATIM 25-01-2010 20:58:34
 OBNUC 1H
 EXMOD single pulse.ex2
 OBFRQ 399.78 MHz
 OBSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 13107
 FREQU 6002.31 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 2.0000 sec
 PW1 4.75 usec
 IRNUC 1H
 CTEMP 19.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.25 Hz
 RGAIN 40

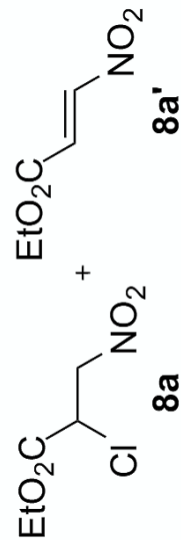
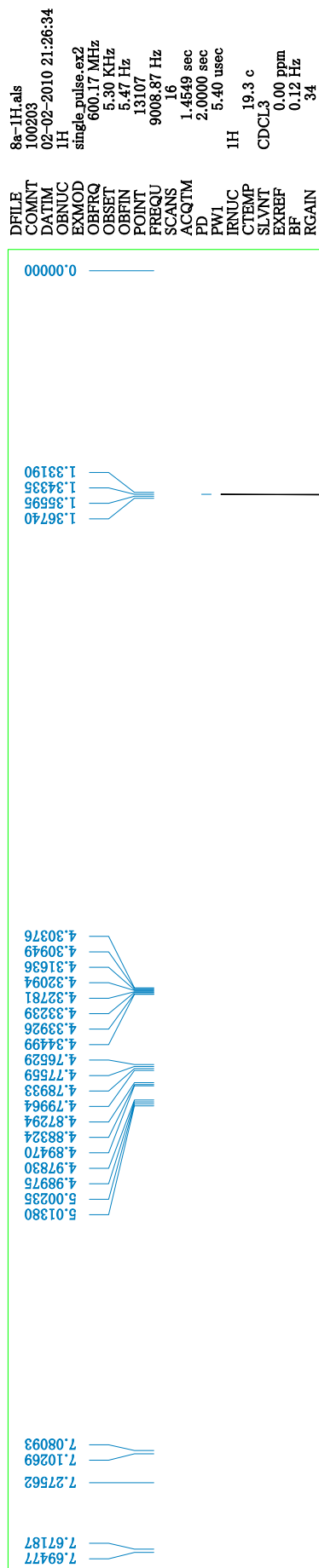


6h (single isomer)

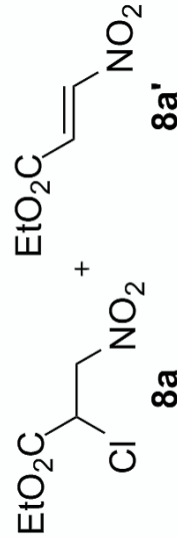
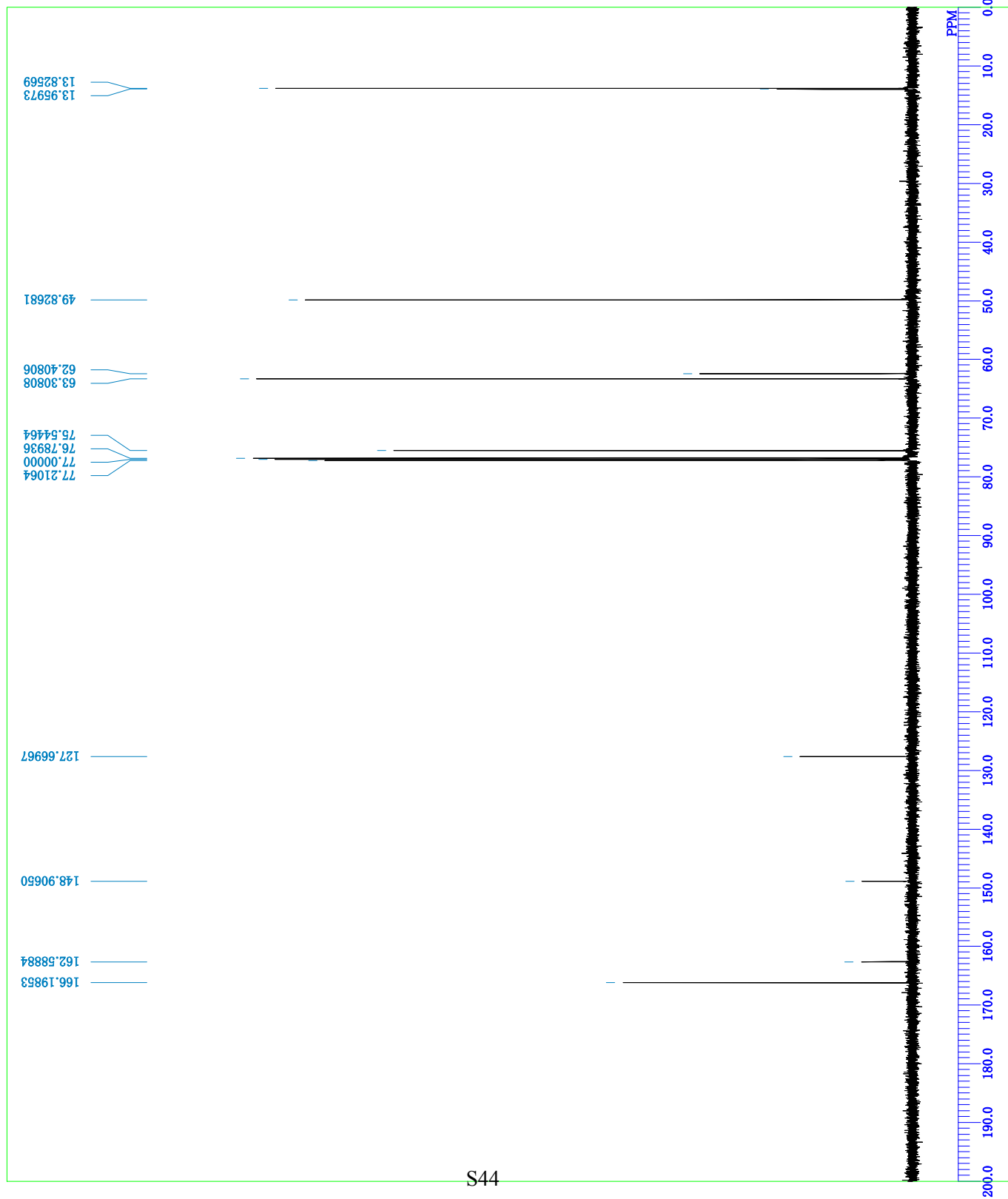
DFILE 6h-C.als
COMNT 100113
DATIM 13-01-2010 21:43:25
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 26214
FREQU 37878.21 Hz
SCANS 686
ACQTM 0.6921 sec
PD 1.2000 sec
PW1 2.77 usec
IRNUC 1H 17.6 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF BF 0.25 Hz
RGAIN 54



6h (single isomer)

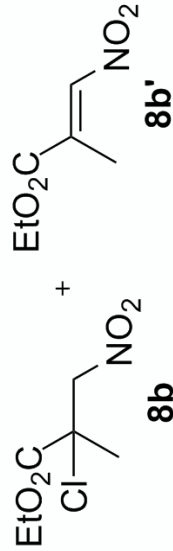
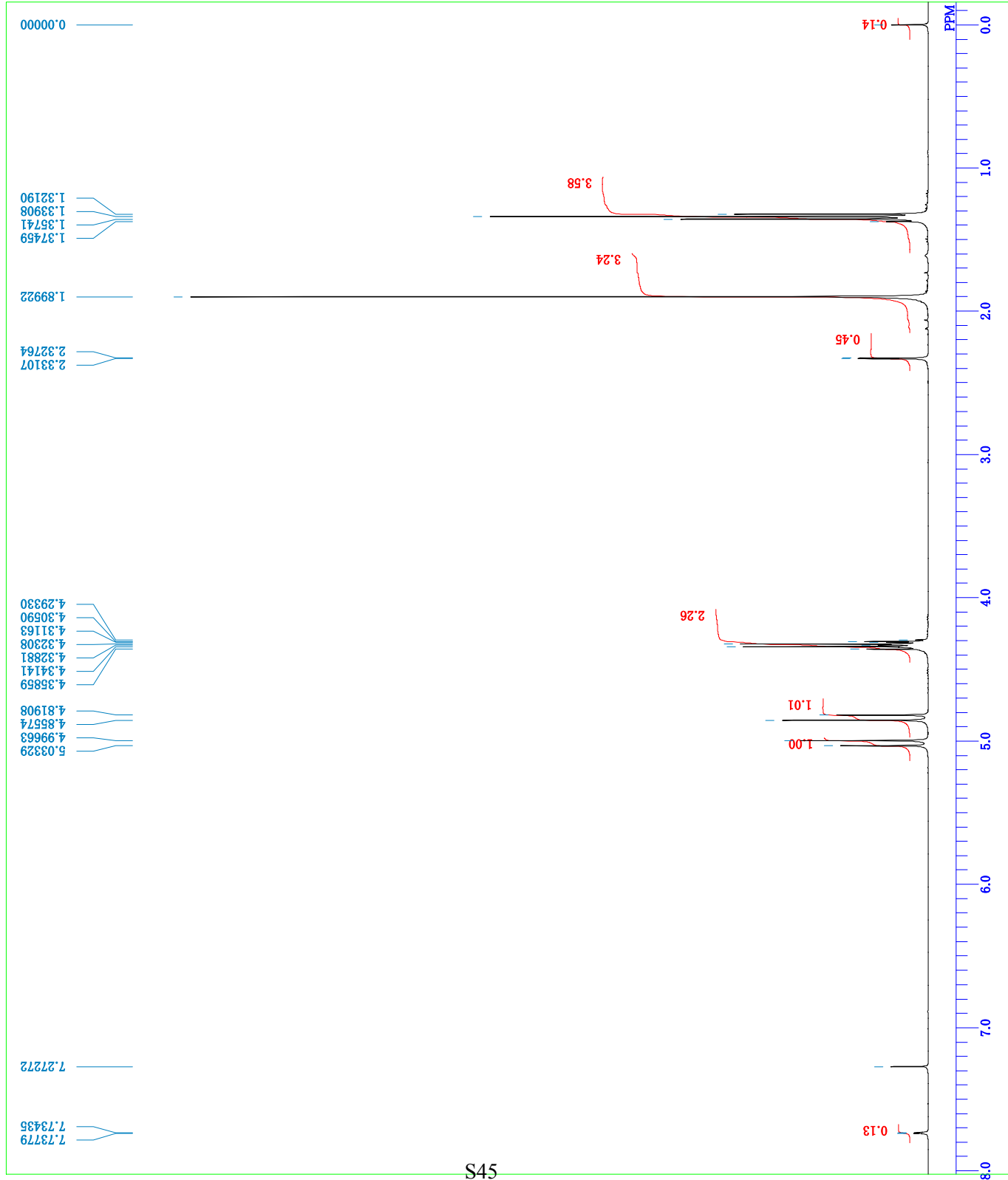


8a-C.als
100203
02-02-2010 21:38:34
13C
single_pulse dec
EXMOD 150.92 MHz
OBFRQ 8.52 KHz
OBSETT 1.74 Hz
POINT 26214
FREQ 37878.21 Hz
SCANS 321
ACQTM 0.6921 sec
PD 1.2000 sec
PW1 2.77 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 54



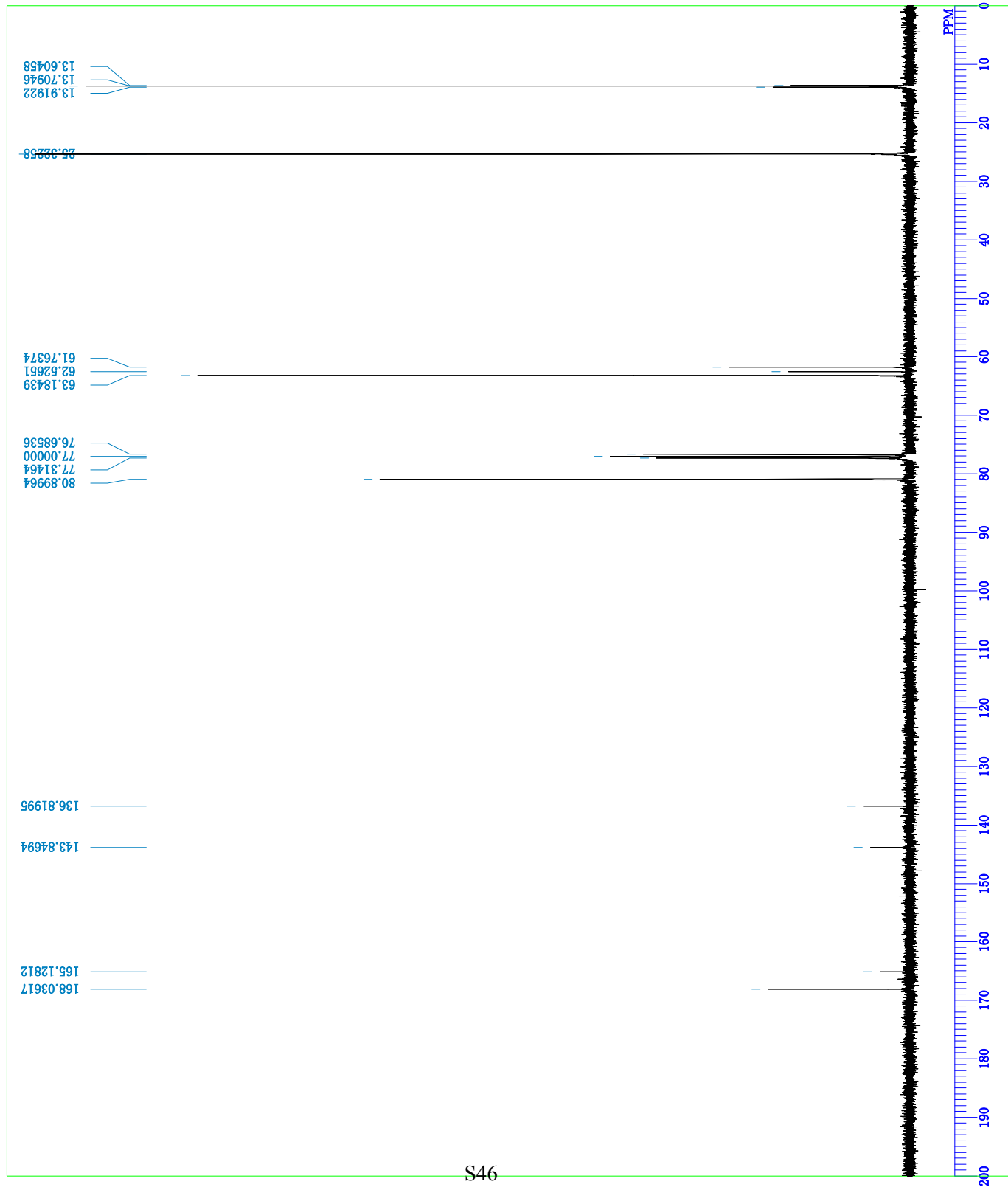
DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFREQ
 OBSETT
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

8b-1H.als
 100118
 18-01-2010 21:07:08
 1H
 single pulse, ex2
 399.78 MHz
 4.19 KHz
 7.29 Hz
 13107
 6002.31 Hz
 16
 2.1837 sec
 2.0000 sec
 4.75 usec
 1H
 18.5 c
 CDCL3
 0.00 ppm
 0.28 Hz
 36



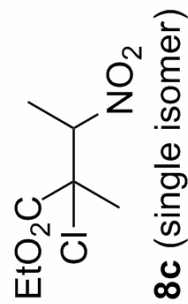
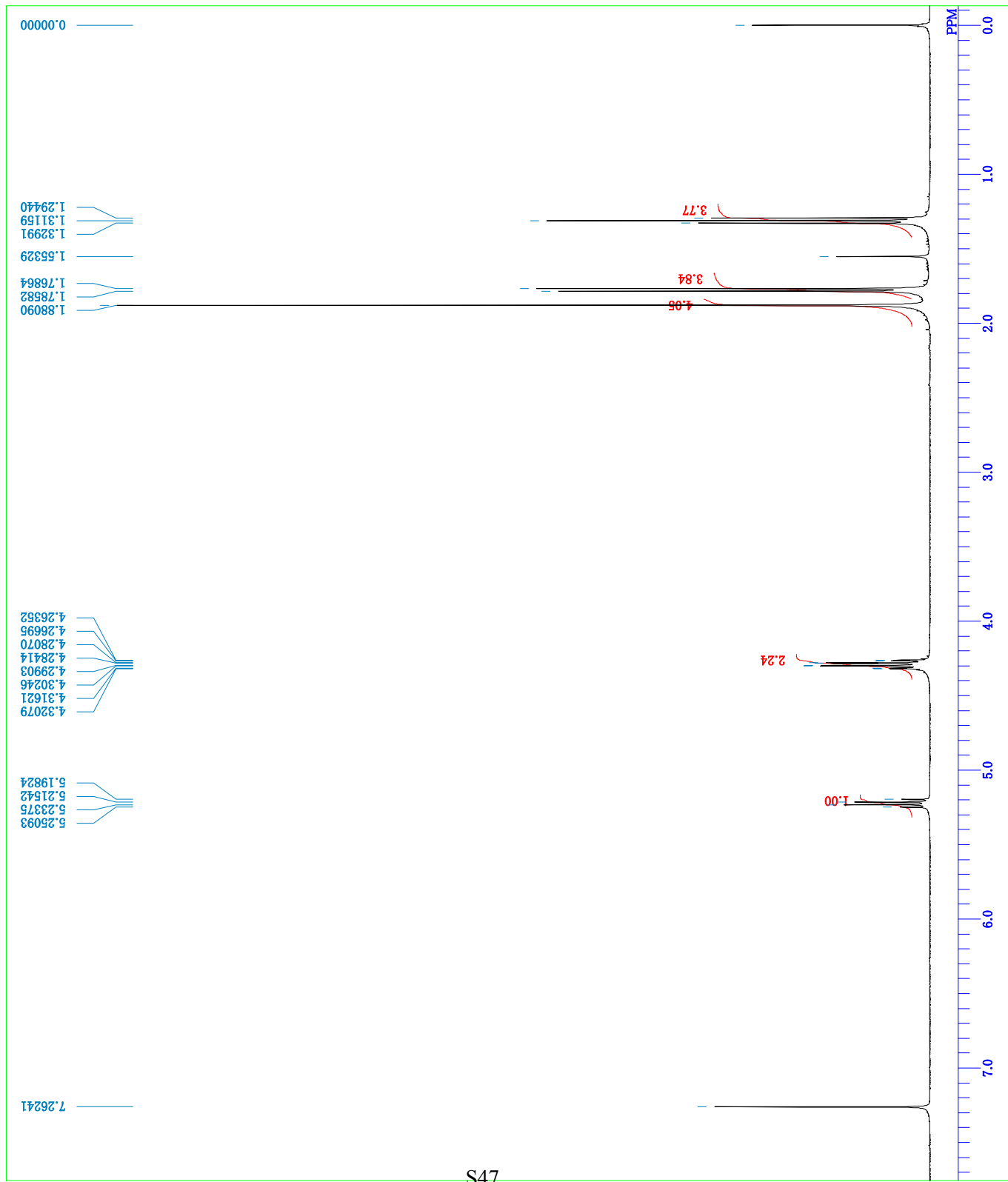
8b-C.als
 100119
 19-01-2010 21:39:41
 13C
 single pulse dec
 100.53 MHz
 5.35 KHz
 5.86 Hz
 26214
 25125.24 Hz
 273
 1.0433 sec
 1.2000 sec
 2.87 usec
 1H 19.3 c
 CDCL3
 77.00 ppm
 0.25 Hz
 60
 RGAIN

DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN



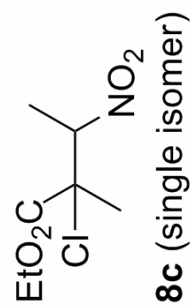
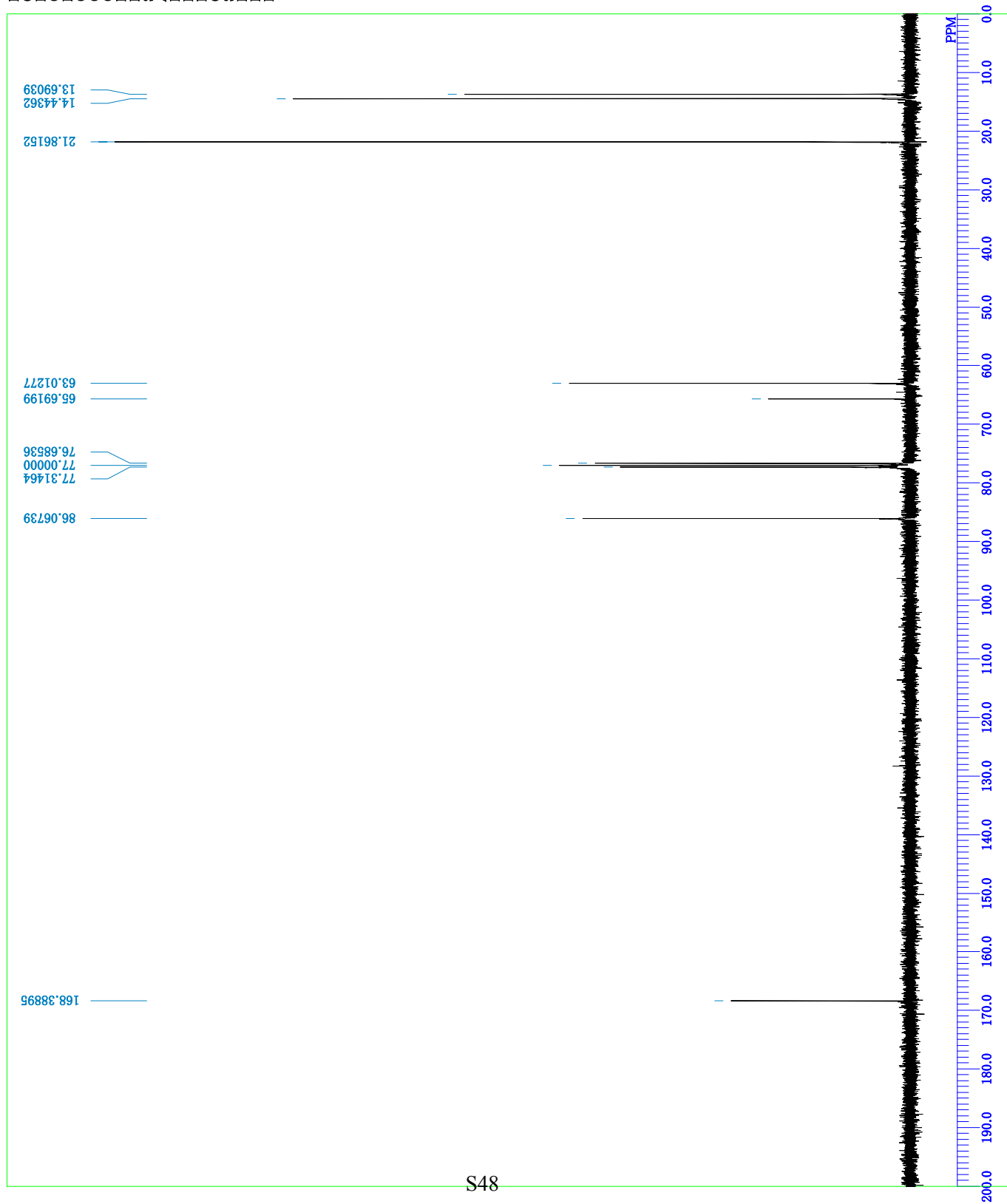
8c-1H.als
100120
20-01-2010 21:51:04
1H
single pulse, ex2
399.78 MHz
4.19 KHz
7.29 Hz
13107
6002.31 Hz
16
2.1837 sec
2.0000 sec
4.75 usec
1H
21.6 c
CDCL3
0.00 ppm
0.25 Hz
46
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFREQ
OBFSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



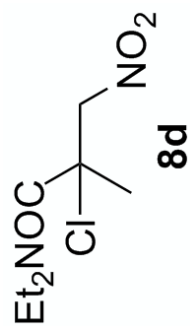
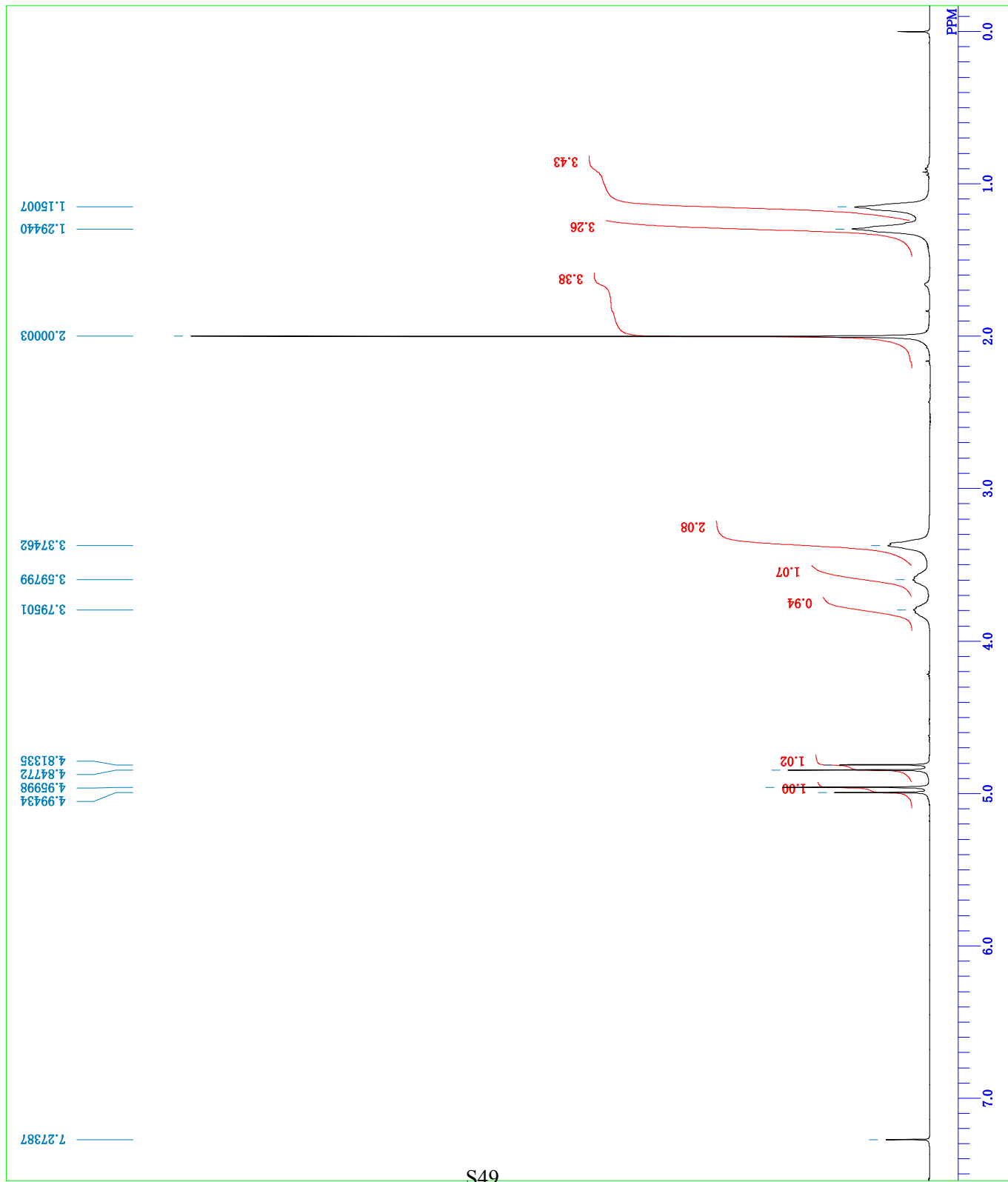
8c-C.als
091214
14-12-2009 22:30:13
13C
single_pulse_dec
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.24 Hz
387
1.0433 sec
1.2000 sec
2.87 usec
1H
20.5 c
CDCL3
77.00 ppm
0.00 Hz
60
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



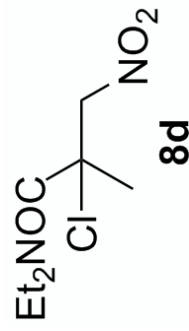
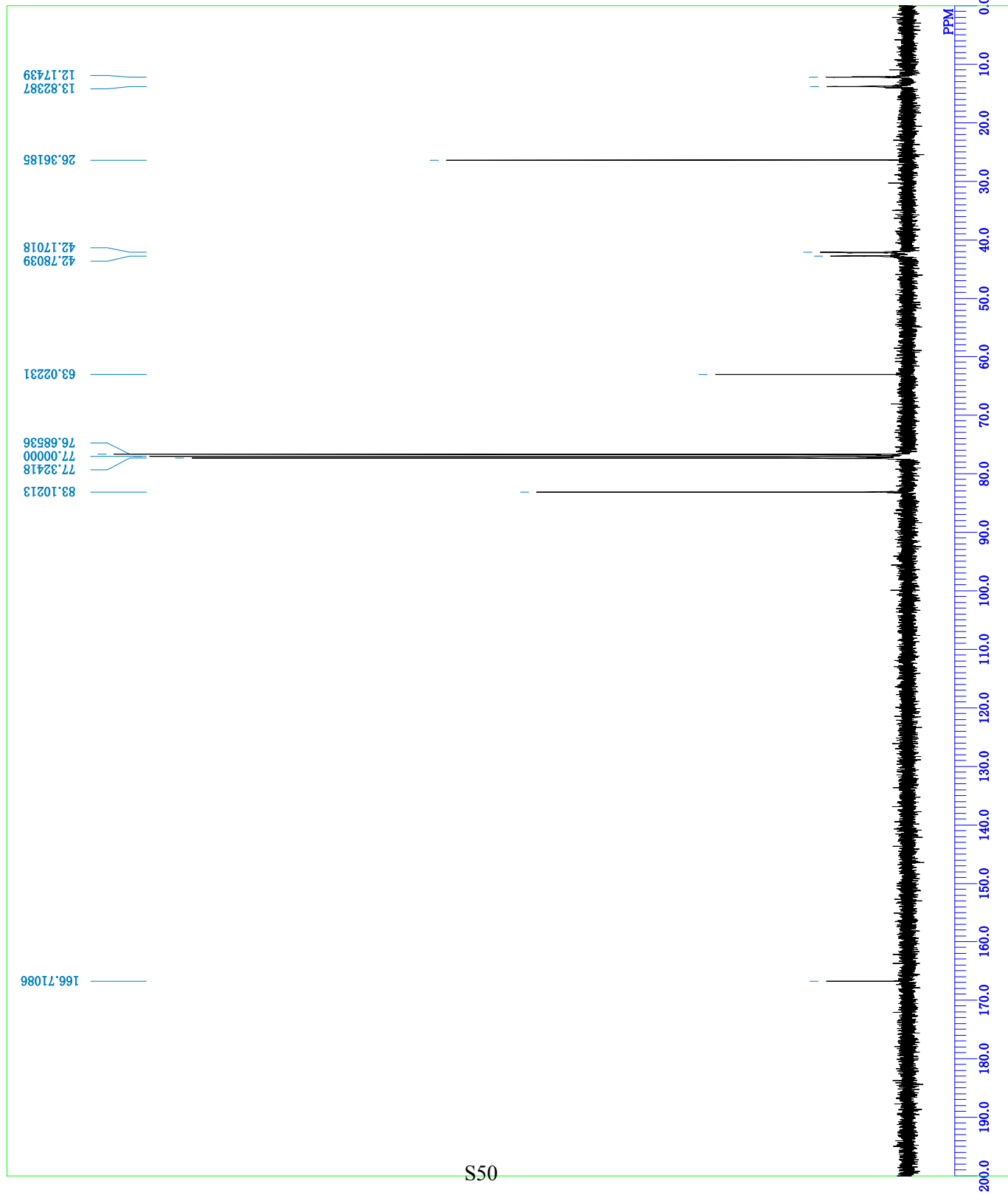
8d-1H.als
100118
18-01-2010 21:23:20
1H
single pulse, ex2
399.78 MHz
4.19 KHz
7.29 Hz
13107
6002.31 Hz
16
2.1837 sec
2.0000 sec
4.75 usec
1H
18.5 c
CDCL3
0.00 ppm
0.28 Hz
34

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PWL
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



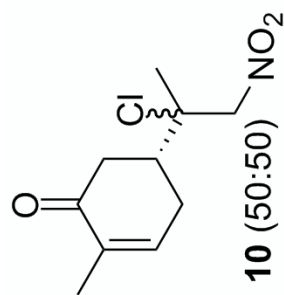
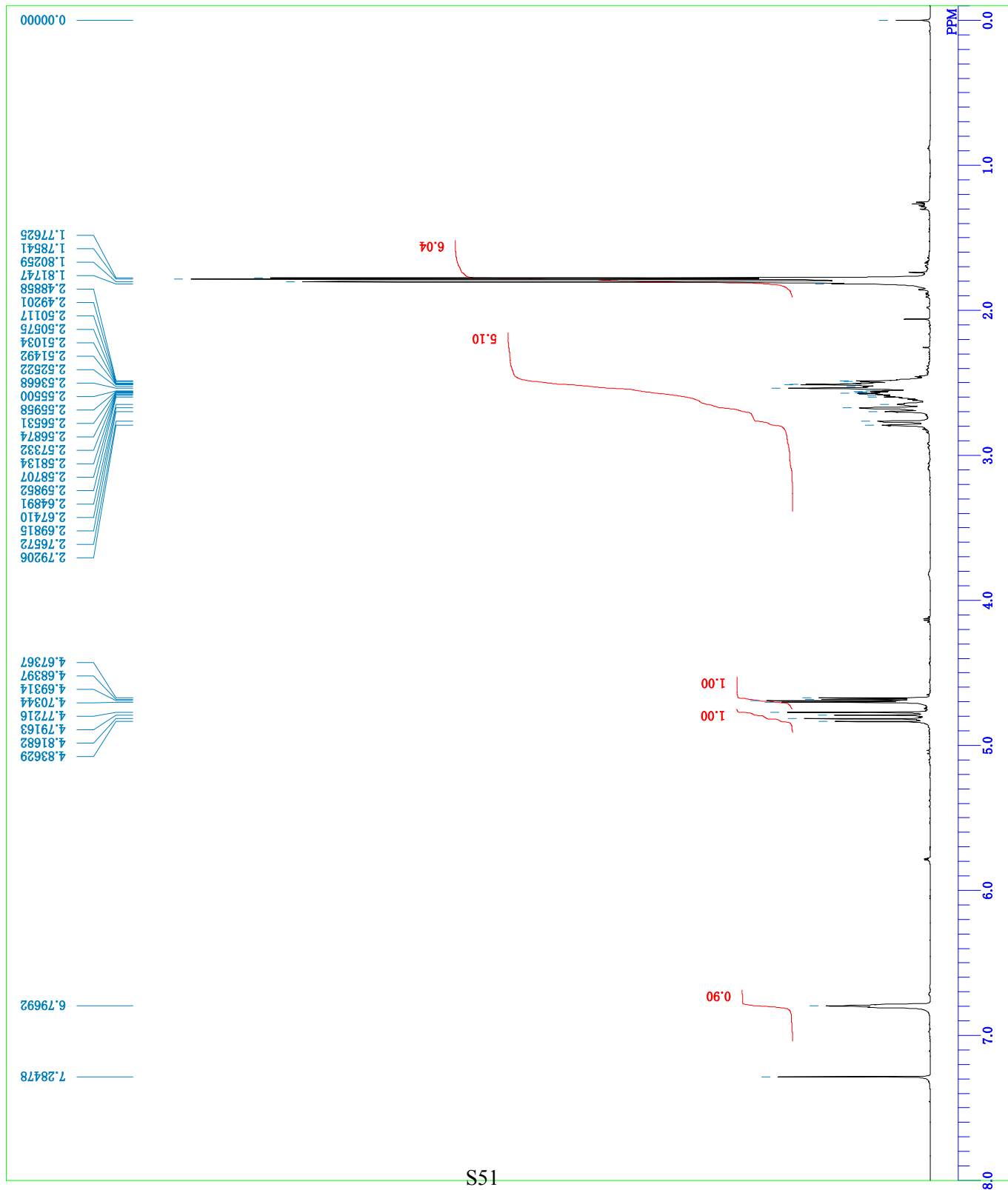
8d-C.als
100118
18-01-2010 21:43:06
13C
single pulse dec
EXMOD 100.53 MHz
OBFRQ 5.35 KHz
OBSET 5.86 Hz
POINT 26214
FREQ 25125.24 Hz
SCANS 514
ACQTM 1.0433 sec
PD 1.2000 sec
PW1 2.87 usec
1H 18.8 c
CDCL3
77.00 ppm
EXREF BF 0.28 Hz
RGAIN 60

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
POINT
FREQ
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



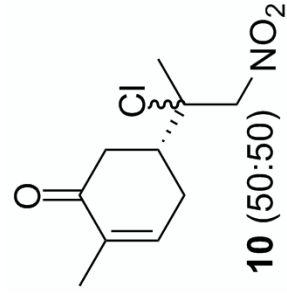
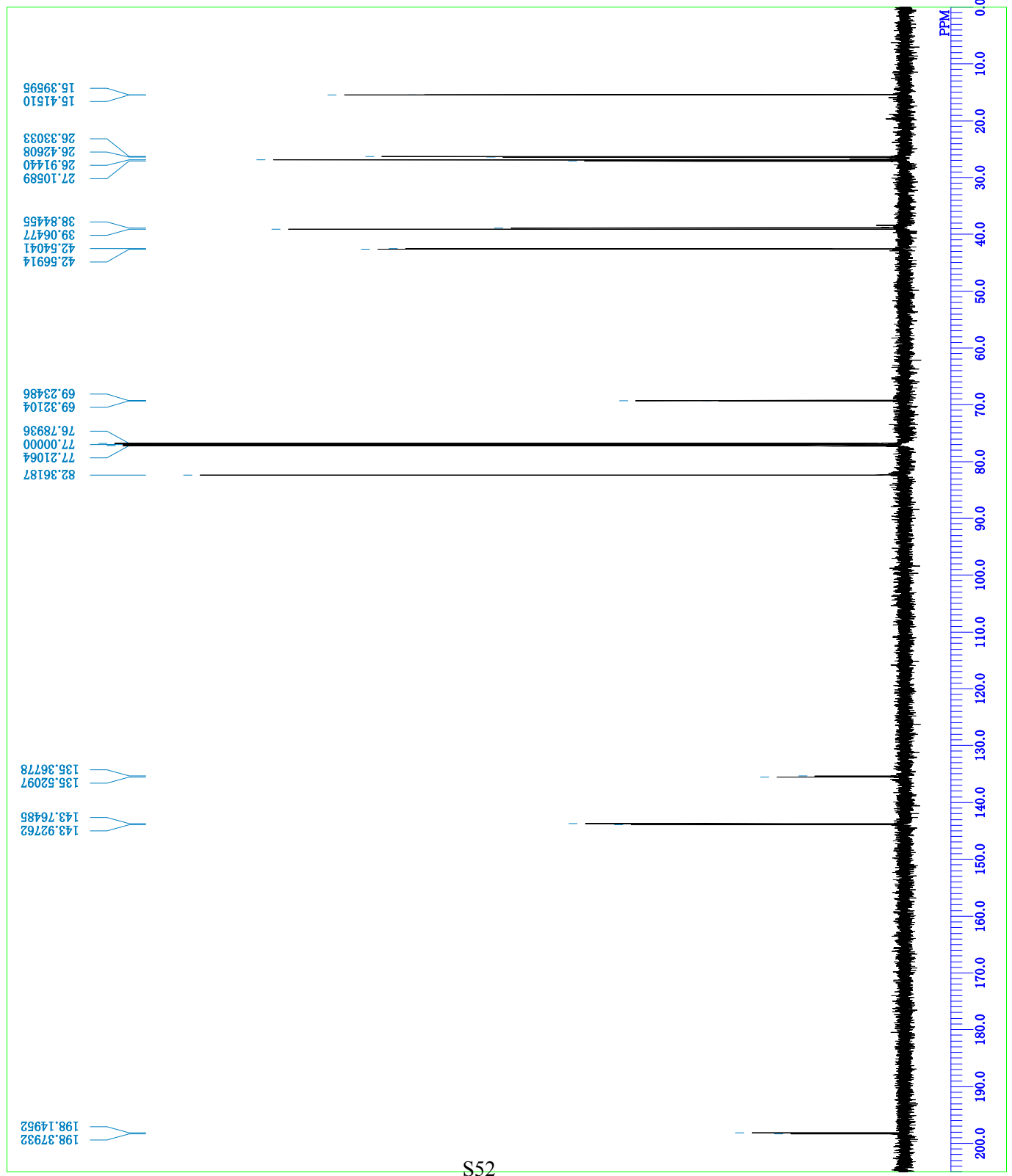
10-1H.als
100224
24-02-2010 21:07:11
1H
single pulse, ex2
600.17 MHz
5.30 KHz
5.47 Hz
13107
9008.87 Hz
16
1.4549 sec
2.0000 sec
6.50 usec
1H
22.2 c
CDCl3
0.00 ppm
0.43 Hz
30
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

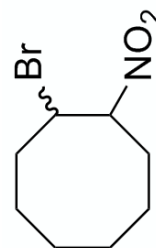
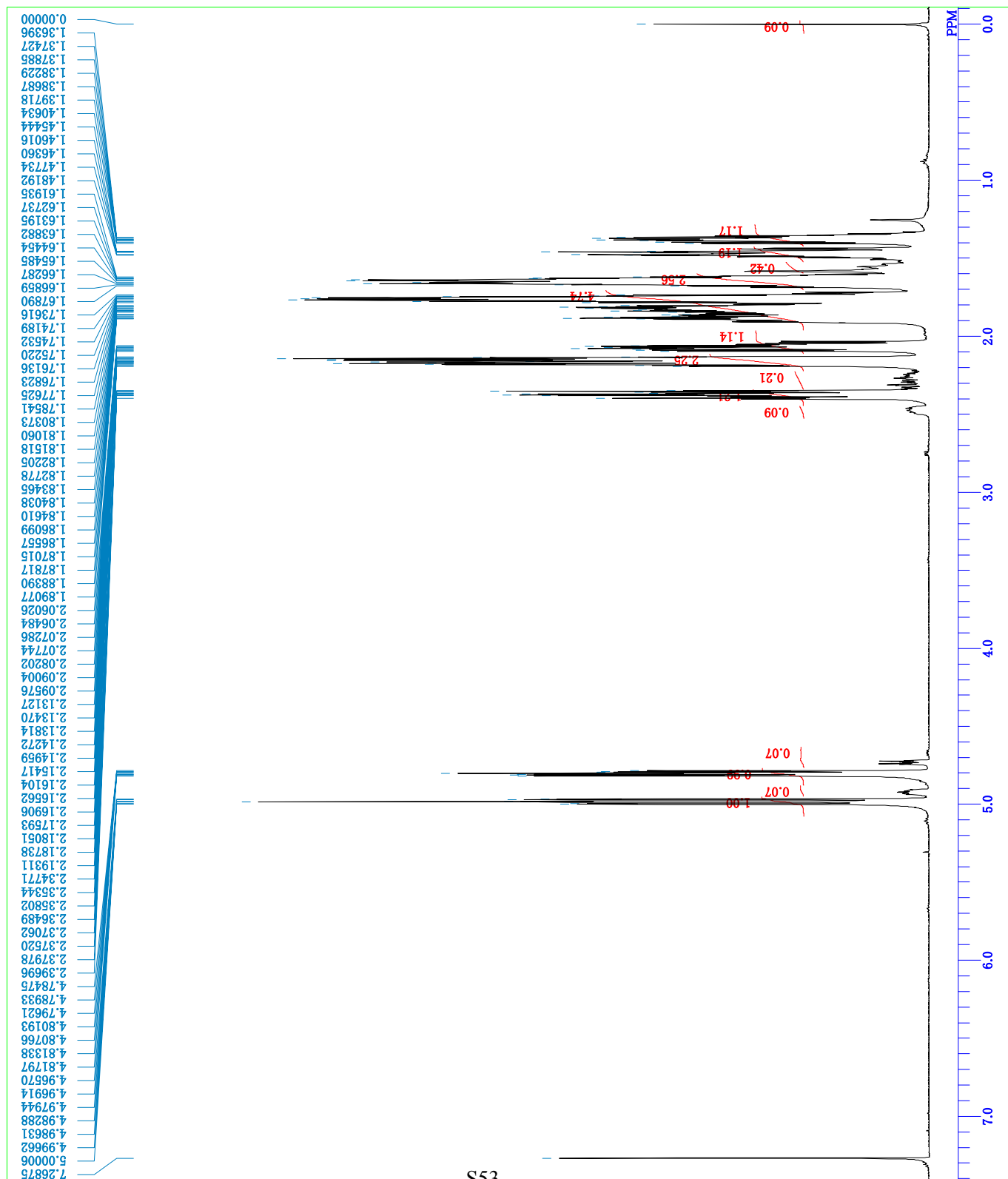


10-C.als
100224
24-02-2010 21:15:46
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
258
0.6921 sec
1.2000 sec
4.00 usec
1H
23.0 c
CDCL3
77.00 ppm
0.43 Hz
56
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



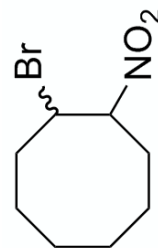
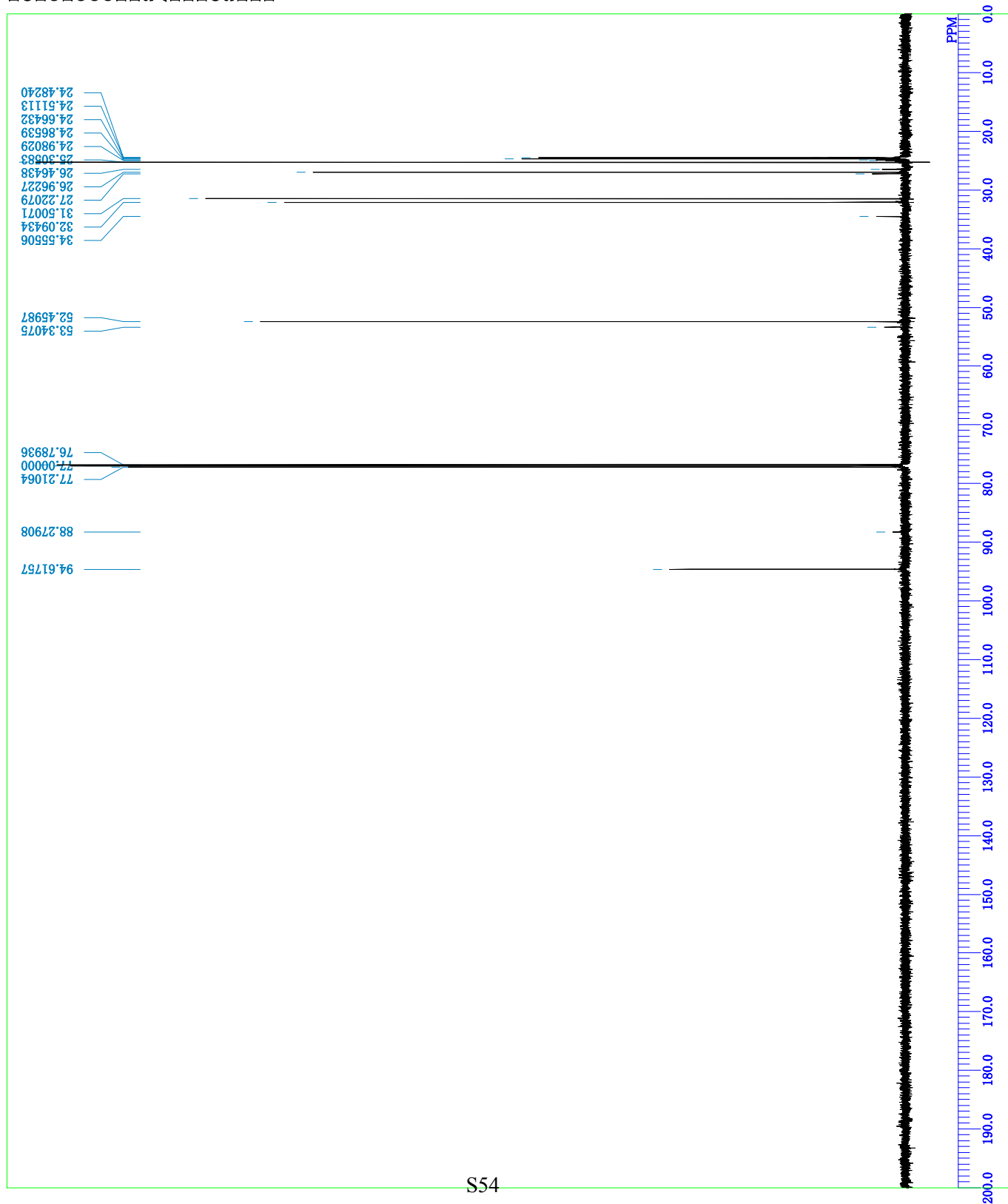
DFILE 13d-1H.hls
 COMINT 100209
 DATIM 09-02-2010 21:49:04
 OBNUC 1H
 EXMOD single pulse, ex2
 OBFRQ 600.17 MHz
 OBSET 5.30 KHz
 OBFIN 5.47 Hz
 POINT 13107
 FREQU 9008.87 Hz
 SCANS 16
 ACQTM 1.4549 sec
 PD 2.0000 sec
 PW1 6.50 usec
 IRNUC 1H
 CTEMP 19.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 34



11d (*trans:cis*, 85:15)

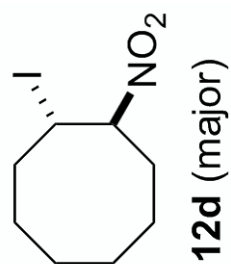
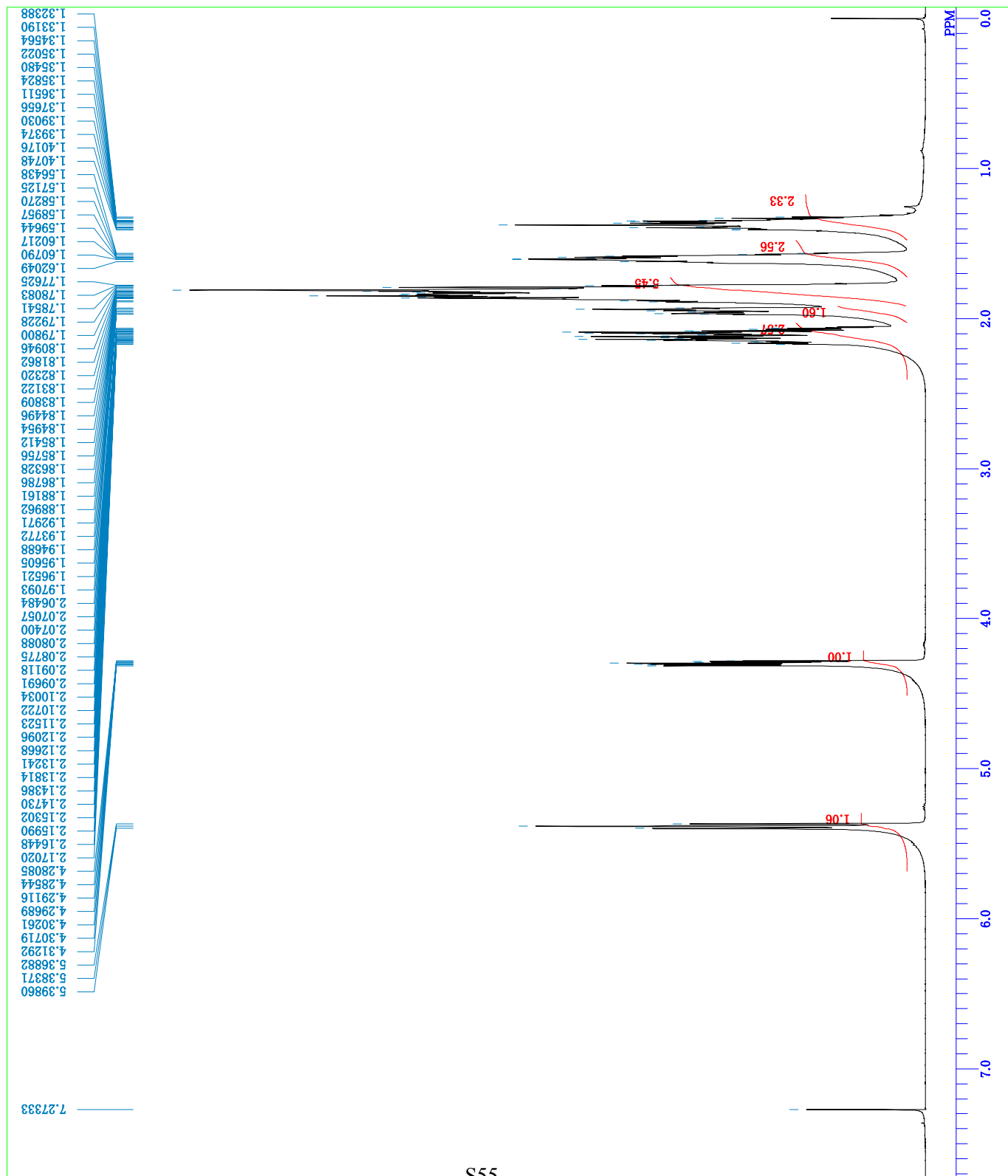
13d-C.als
100210
10-02-2010 21:49:58
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
781
0.6921 sec
1.2000 sec
4.00 usec
1H 19.9 c
CDCL3
77.00 ppm
0.12 Hz
56
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



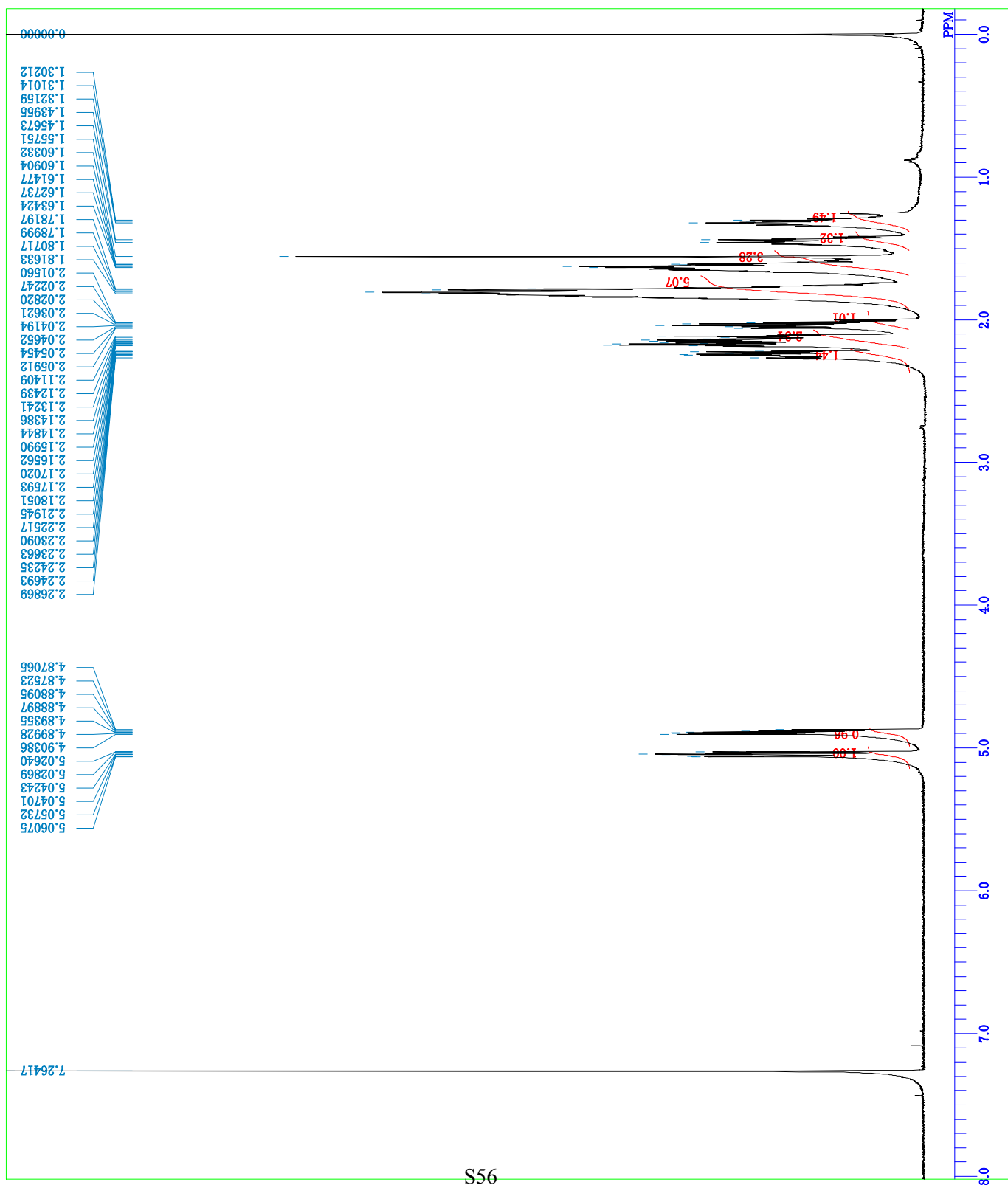
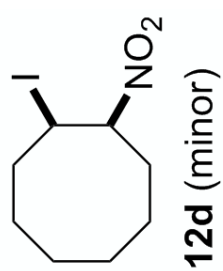
11d (*trans:cis*, 85:15)

DFILE 100208
 COMINT 08-02-2010 20:54:22
 DATIM 1H
 OBNUC single pulse, ex2
 EXMOD 600.17 MHz
 OBFRQ 5.30 KHz
 OBSET 5.47 Hz
 OBFIN 13107
 POINT 9008.87 Hz
 FREQU 16
 SCANS 1.4549 sec
 ACQTM 2.0000 sec
 PD 6.50 usec
 PW1 1H
 IRNUC 18.9 c
 CTEMP CDCL3
 SLVNT 0.00 ppm
 EXREF BF
 RGAIN 28

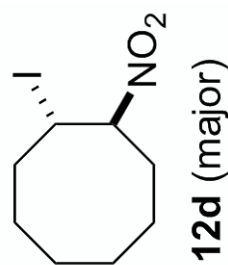
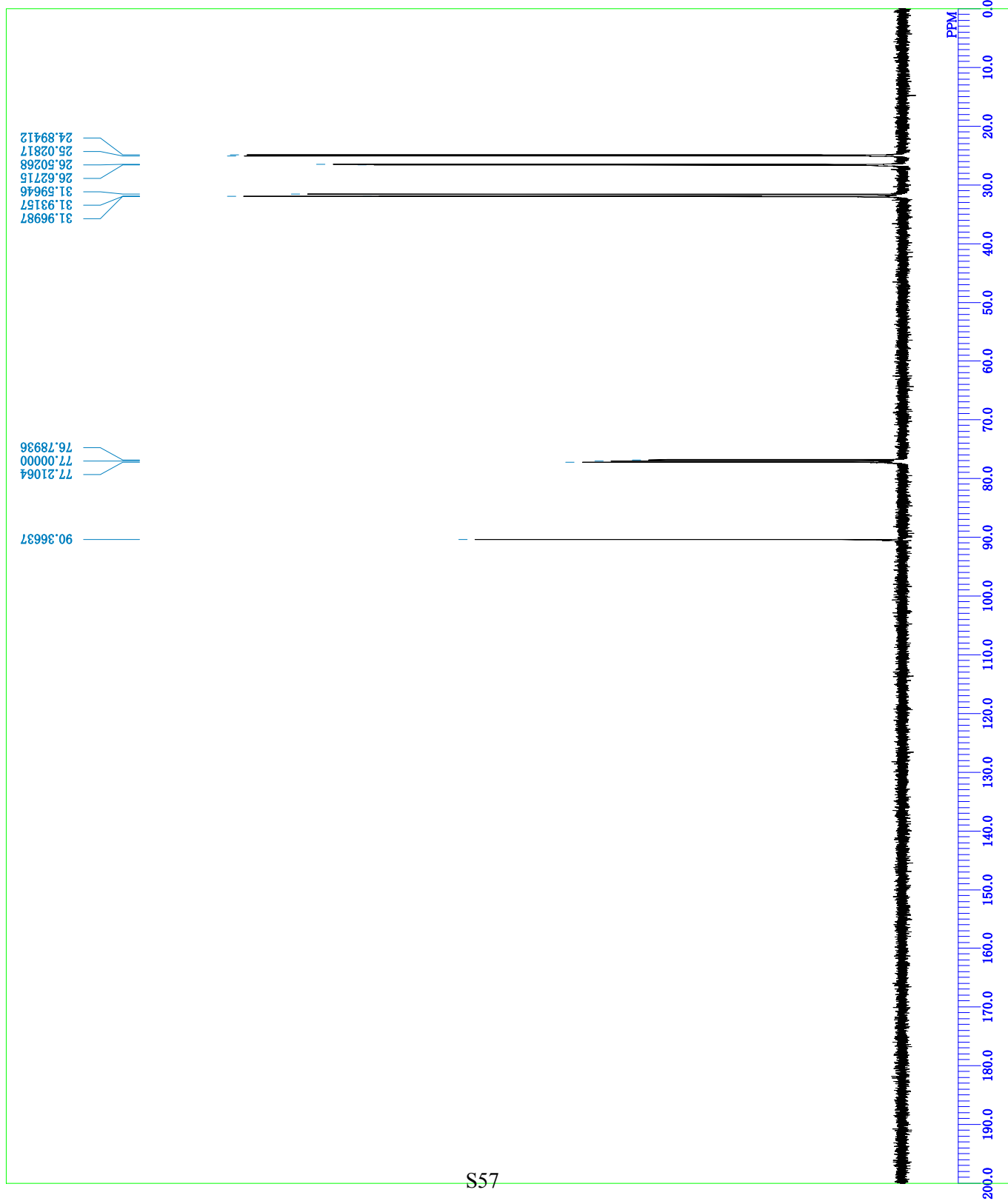


DFILE
 COMINT
 DATIM
 OBNUC
 EXMOD
 OBFRQ
 OBSET
 OBFIN
 POINT
 FREQU
 SCANS
 ACQTM
 PD
 PW1
 IRNUC
 CTEMP
 SLVNT
 EXREF
 BF
 RGAIN

14e-minor-Hals
 100210
 10-02-2010 21:04:25
 1H
 single_pulse.ex2
 600.17 MHz
 5.30 KHz
 5.47 Hz
 13107
 9008.87 Hz
 16
 1.4549 sec
 2.0000 sec
 6.50 usec
 1H
 19.0 c
 CDCL3
 0.00 ppm
 0.12 Hz
 44

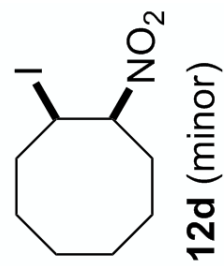
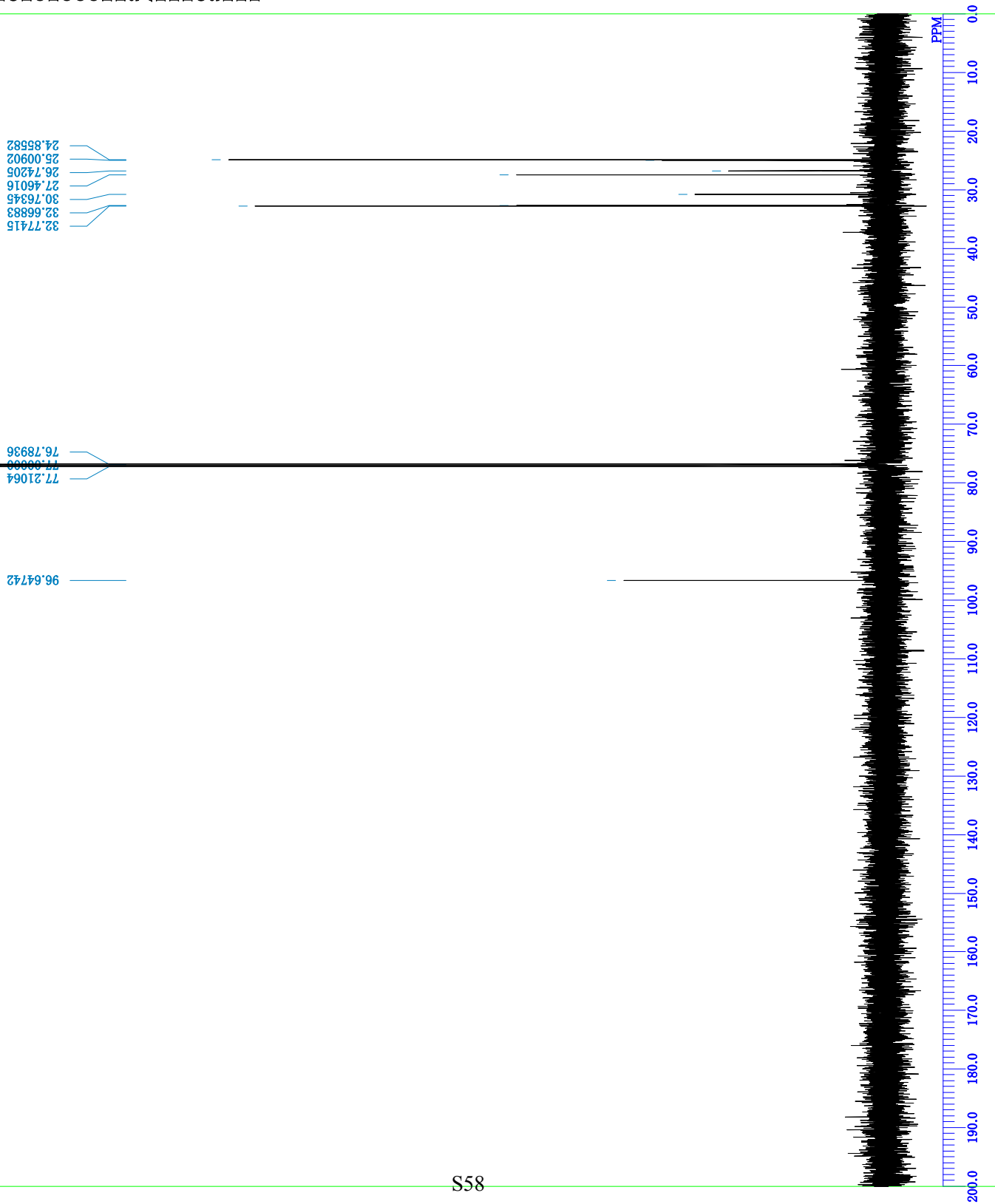


DFILE 14e-major-C.als
 COMINT 100208
 DATIM 08-02-2010 21:03:00
 OBNUC ¹³C
 single pulse dec
 OBFRQ 150.92 MHz
 OBSET 8.52 KHz
 OBFIN 1.74 Hz
 POINT 26214
 FREQU 37878.21 Hz
 SCANS 258
 ACQTM 0.6921 sec
 PD 1.2000 sec
 PW1 4.00 usec
 IHN 1H
 CTEMP 19.7 c
 SLYNT CDCL₃
 EXREF 77.00 ppm
 BF 0.08 Hz
 RGAIN 56

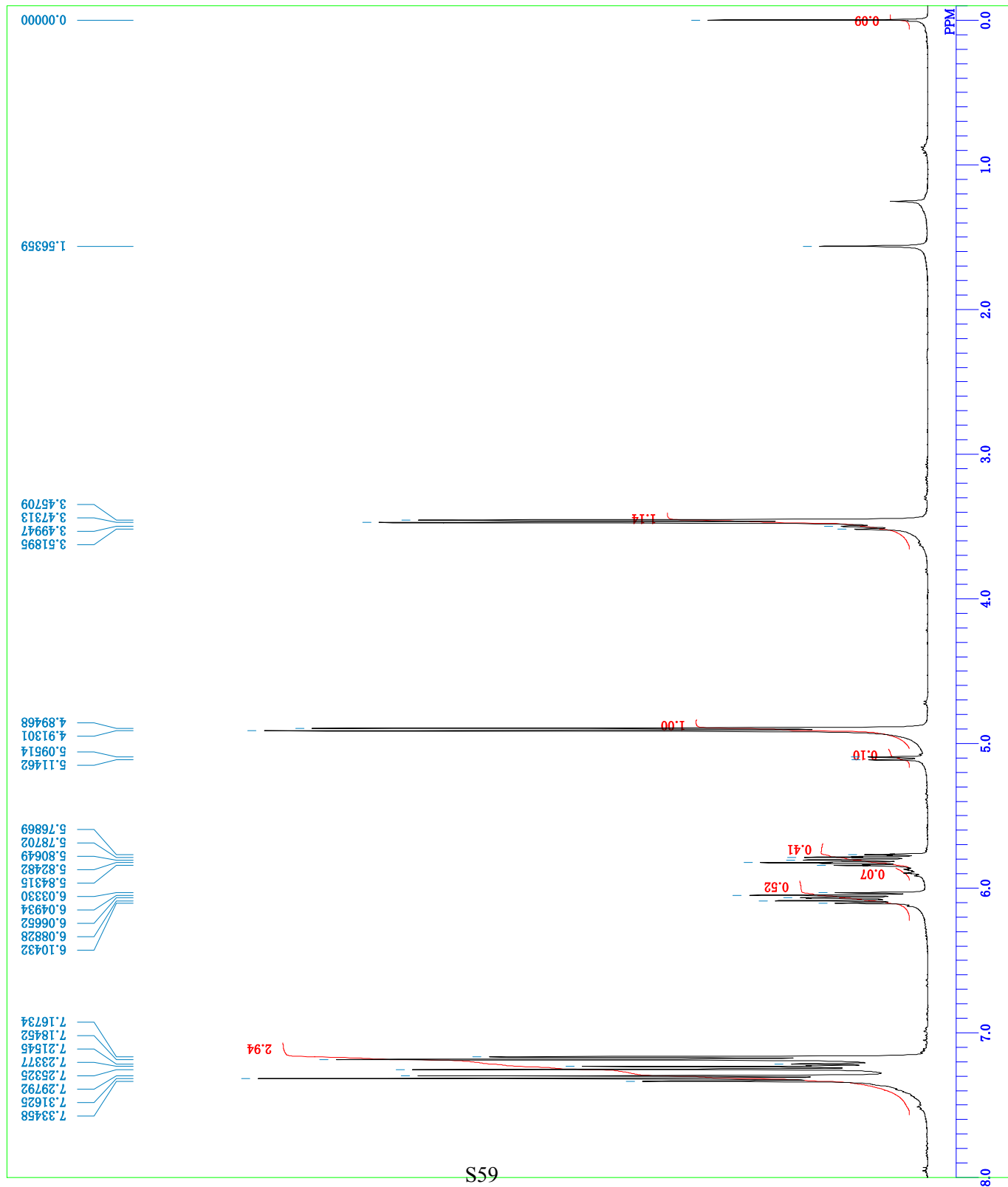


14e-minor-C.als
100209
09-02-2010 21:44:32
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
102
0.6921 sec
1.2000 sec
4.00 usec
1H 19.8 c
CDCL3
77.00 ppm
0.12 Hz
56
RGAIN

DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



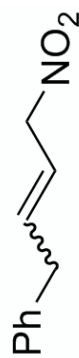
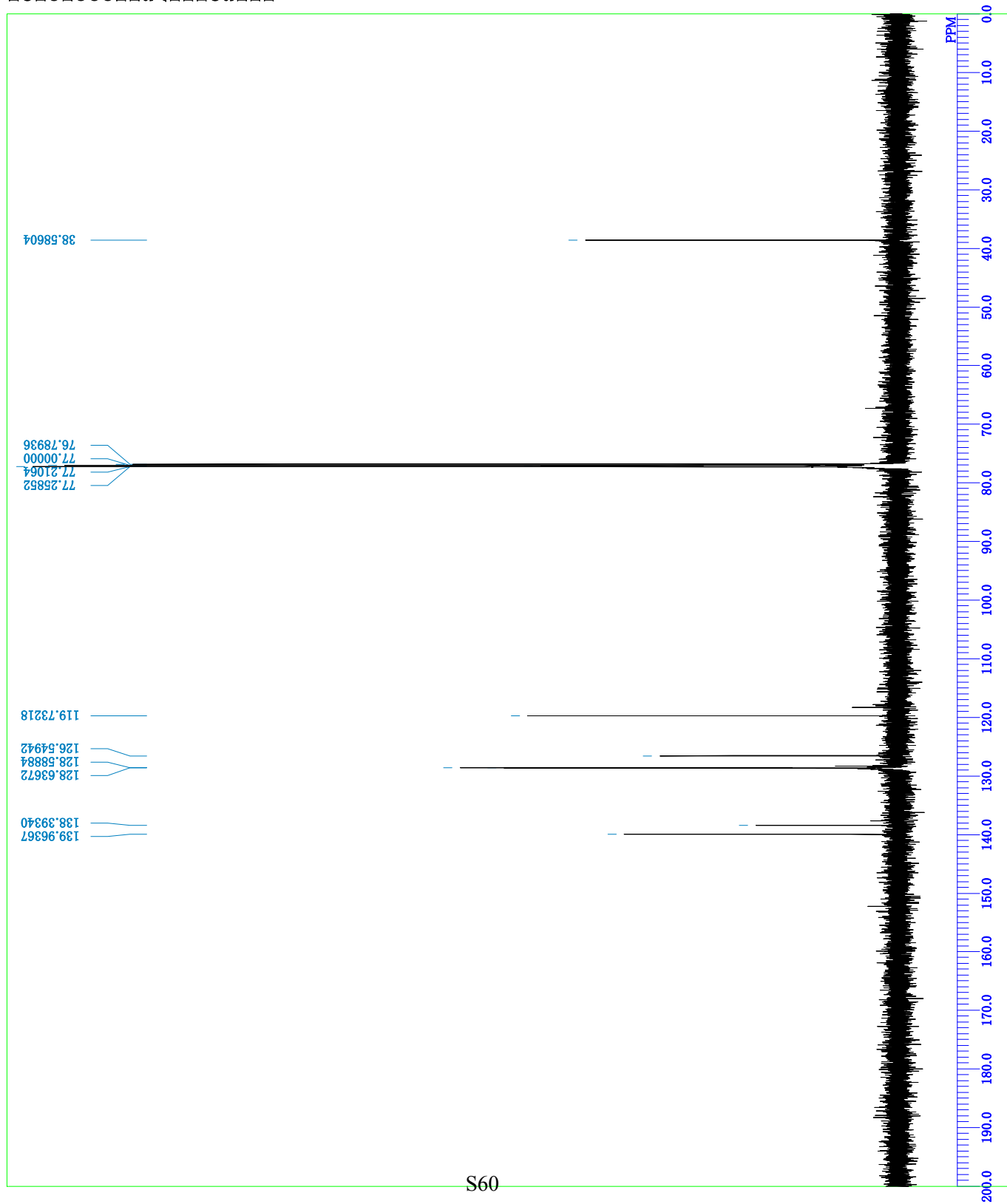
16-1H.als
100115
15-01-2010 19:36:22
1H
single pulse, ex2
399.78 MHz
4.19 KHz
7.29 Hz
13107
6002.31 Hz
16
2.1837 sec
2.0000 sec
4.75 usec
1H 17.3 c
CDCL3
0.00 ppm
0.25 Hz
40
RGAIN



14 (E:Z, 91:9)

16-C.als
100114
14-01-2010 21:20:47
13C
single pulse dec
150.92 MHz
8.52 KHz
1.74 Hz
26214
37878.21 Hz
258
0.6921 sec
1.2000 sec
2.77 usec
1H 17.2 c
CDCL3
77.00 ppm
0.12 Hz
52
RGAIN

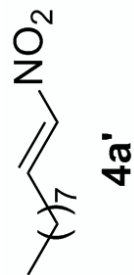
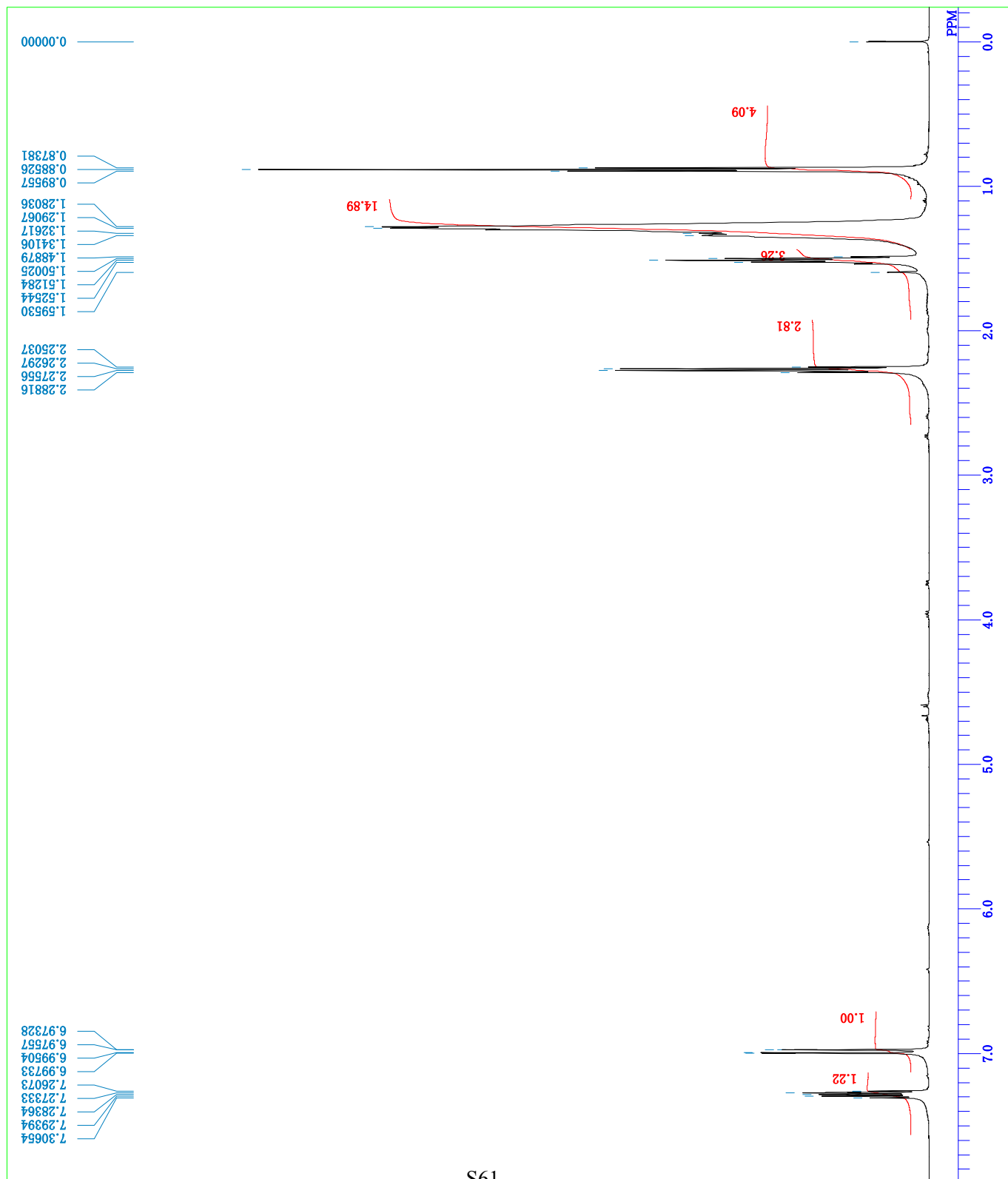
DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

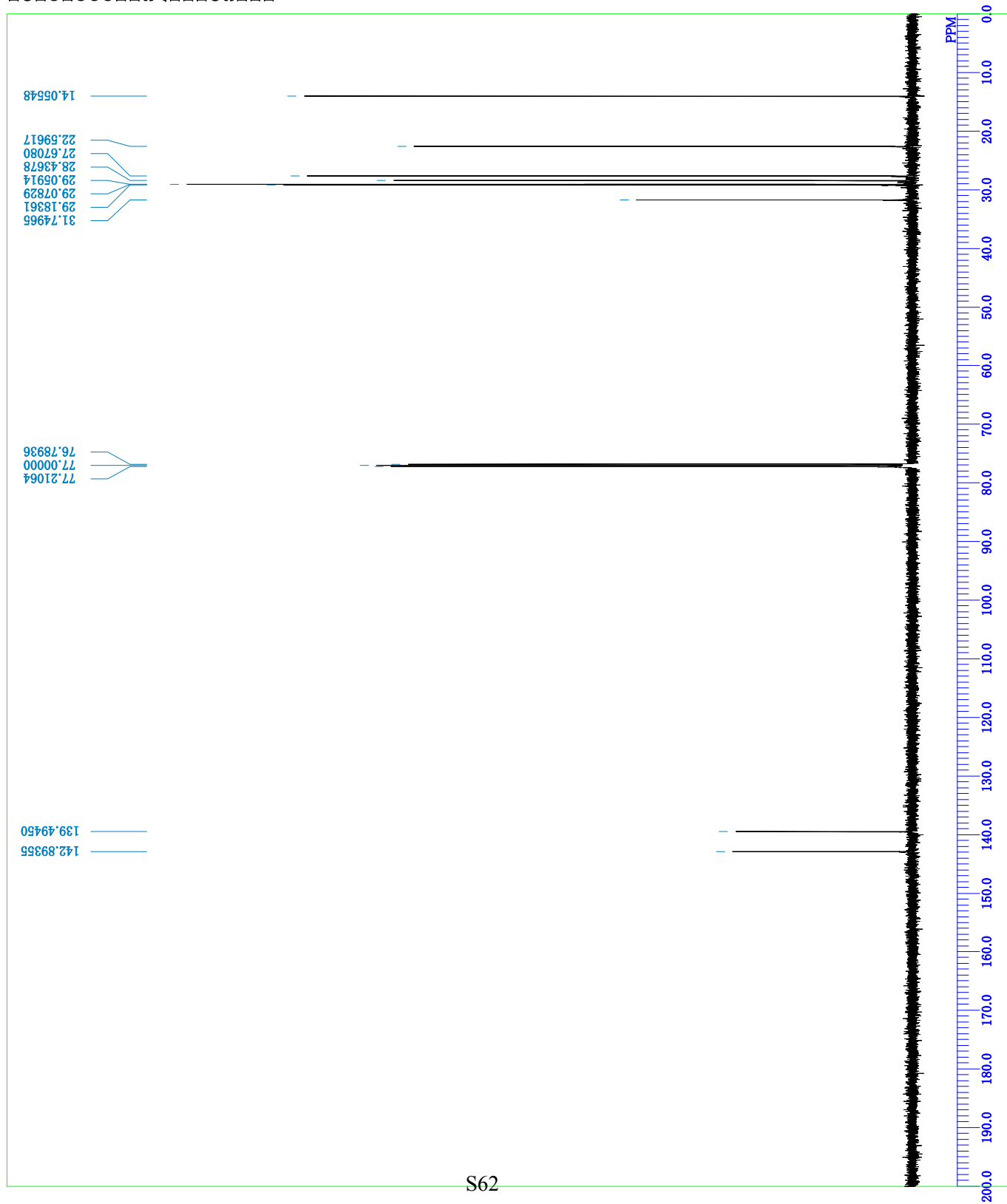


14 (E:Z, 91:9)

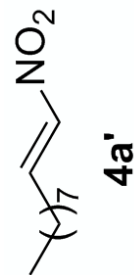
4a'(elim)-1H.als
100114
14-01-2010 21:27:52
1H
single pulse, ex2
600.17 MHz
5.30 KHz
5.47 Hz
13107
9008.87 Hz
16
1.4549 sec
2.0000 sec
5.40 usec
1H 16.7 c
CDCL3
0.00 ppm
0.12 Hz
30
RGAIN

DFILE
COMINT
DATUM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



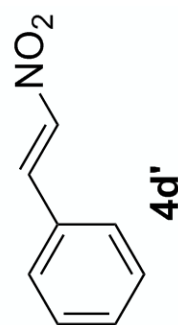
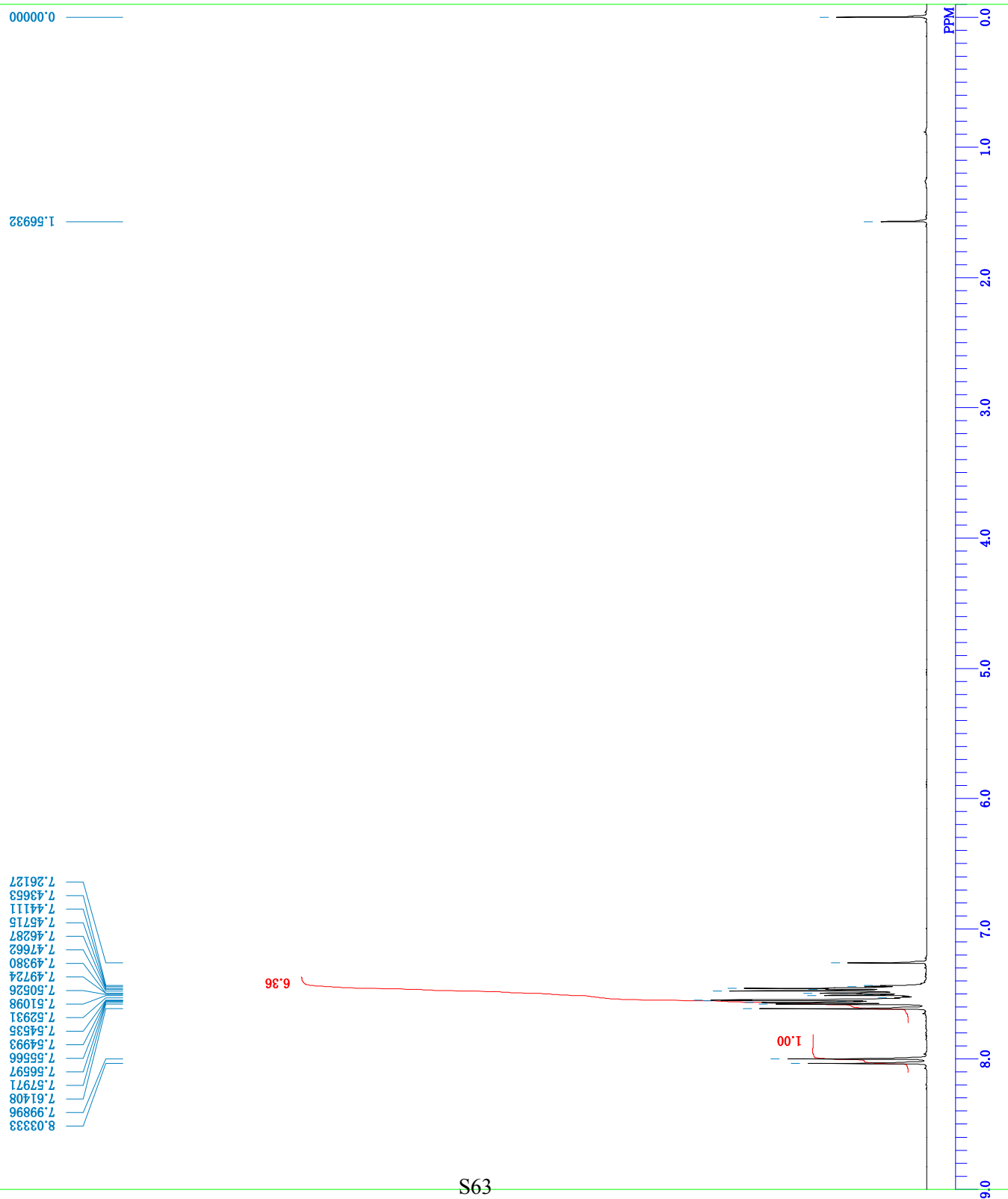


DFILE	4a*(elim)-C.dls
COMNT	100114
DATIM	14-01-2010 21:36:38
EXMOD	13C
EXNUM	single pulse, dec
OBFRQ	150.92 MHz
OBFSZ	8.52 KHz
OBFT	1.74 Hz
POINT	26214
POINT	37878-21 Hz
FREQU	260
SCANS	0.6921 sec
ACQTM	1.9006 sec
PD	2.77 usec
PW1	1H
IRNUC	17.3 °C
CTEMP	CDCL3
SLVNT	77.00 ppm
EXREF	0.12 Hz
BF	54
RGAIN	54



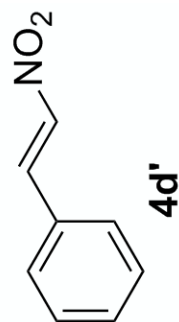
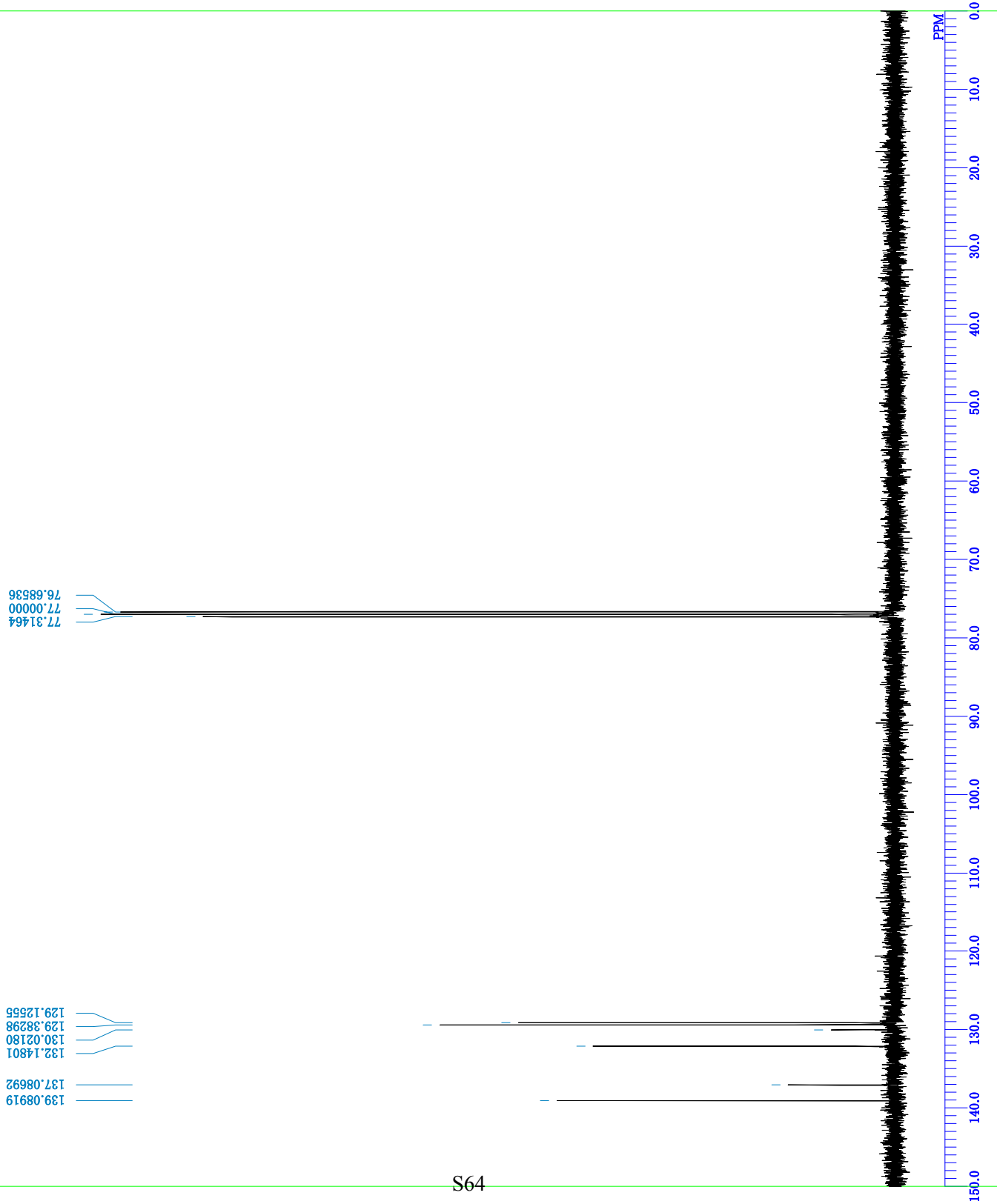
4d'(elim)-1H.als
100126
26-01-2010 21:27:59
1H
single pulse, ex2
399.78 MHz
4.19 KHz
7.29 Hz
13107
6002.31 Hz
16
2.1837 sec
2.0000 sec
4.75 usec
1H 19.3 c
CDCL3
0.00 ppm
0.25 Hz
44
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



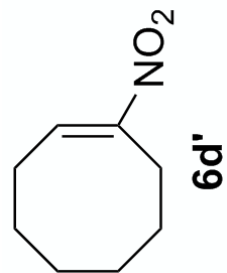
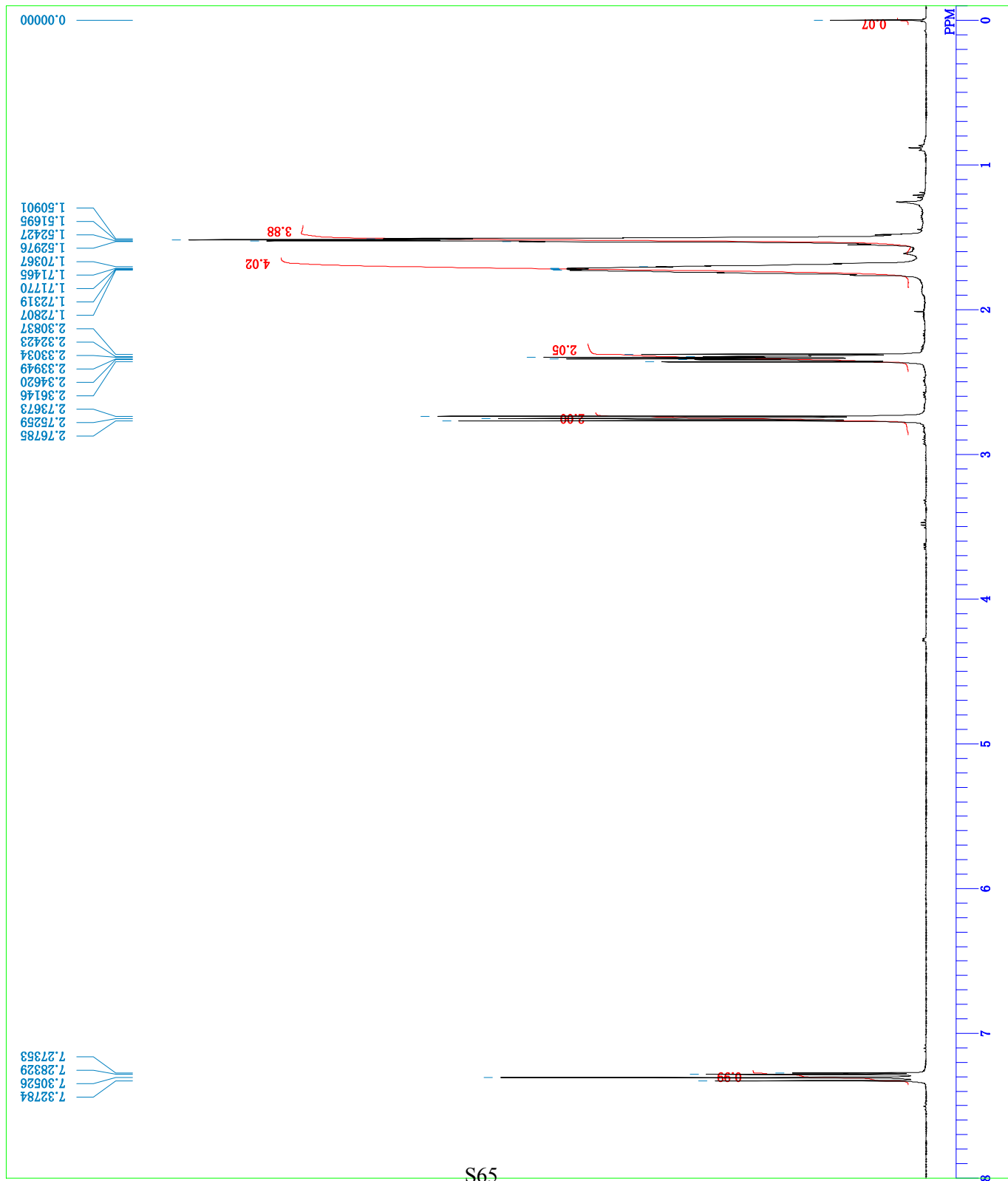
4d'(elim)-C.als
100126
26-01-2010 21:38:12
13C
single pulse dec
100.53 MHz
5.35 KHz
5.86 Hz
26214
258
25125.24 Hz
1.0433 sec
1.2000 sec
2.87 usec
1H 19.5 c
CDCL3
77.00 ppm
0.25 Hz
60
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



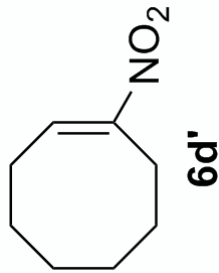
6d'(elim)-1H.als
091205
Sat Dec 05 14:53:26 2009
1H
non
399.65 MHz
0.00 KHz
134300.00 Hz
32768
7993.60 Hz
16
4.0993 sec
2.9007 sec
6.80 usec
1H
22.3 c
CDCl3
0.00 ppm
0.12 Hz
18
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



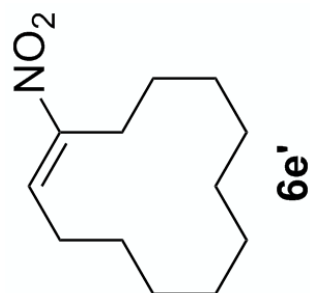
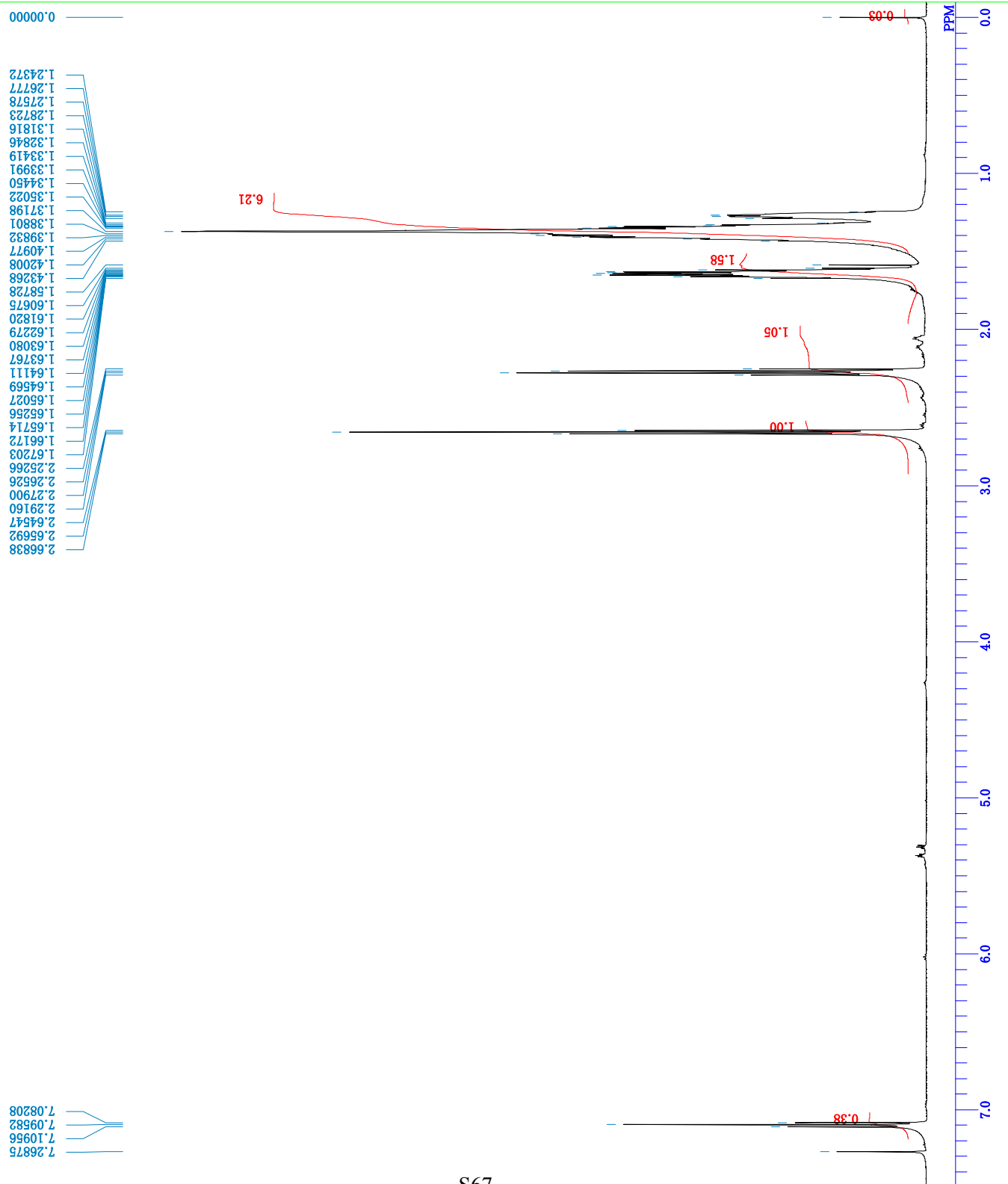
6d'(elim)-C.als
091205
Sat Dec 05 15:07:00 2009
13C
bcm
100.40 MHz
0.00 KHz
135500.00 Hz
32768
27100.27 Hz
257
1.2091 sec
1.7909 sec
4.90 usec
1H
22.5 c
CDCL3
77.00 ppm
0.12 Hz
27
RGAIN

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



6e' (elim)-1H.als
100206
06-02-2010 15:45:11
1H
single_pulse.ex2
600.17 MHz
5.30 KHz
5.47 Hz
13107
9008.87 Hz
16
1.4549 sec
2.0000 sec
6.50 usec
1H
18.8 c
CDCL3
0.00 ppm
0.12 Hz
30

DFILE
COMINT
DATIM
OBNUC
EXMOD
OBFREQ
OBSETT
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN



DFILE COMINT
DATIM 06-02-2010 15:56:53
OBNUC 13C
EXMOD single_pulse dec
OBFRQ 150.92 MHz
OBSETT 8.52 KHz
OBFIN 1.74 Hz
POINT 26214
FREQU 37878.21 Hz
SCANS 357
ACQTM 0.6921 sec
PD 1.2000 sec
PW1 4.00 usec
IRNUC 1H 19.6 c
CTEMP CDCL3
SLVNT 77.00 ppm
EXREF BF 0.12 Hz
RGAIN 56

